MOLECULAR PHYSICS

An international journal in the field of chemical physics

CUMULATIVE INDEX OF AUTHORS

With Titles of Papers

VOLUMES 61–80 (1987–1993)

Prepared by Dr. B. J. HOWARD

EDITORS
Professor H. F. SCHAEFER III (Chairman)
Dr. G. JACKSON
Professor N. C. HANDY
Professor I. M. MILLS

Taylor & Francis
London • New York • Philadelphia

MOLECULAR PHYSICS

An international journal in the field of chemical physics

Editors

Professor H. F. SCHAEFER III (Chairman)
Center for Computational Quantum Chemistry,
University of Georgia,
Athens, Georgia 30602, USA

Dr. G. JACKSON
Department of Chemistry,
University of Sheffield,
Sheffield S3 7HF

Professor N. C. HANDY
Department of Chemistry,
University of Cambridge,
Lensfield Road,
Cambridge CB2 1EW

Executive Committee

Editors: R. F. Barrow, *Oxford*; D. Clary, *Cambridge*; R. N. Dixon, *Bristol*; R. Evans, *Bristol*; G. R. Fleming, *Chicago*; B. J. Howard, *Oxford*; R. M. Lynden-Bell, *Cambridge*; I. R. McDonald, *Cambridge*; K. A. McLauchlan, *Oxford*; P. A. Madden, *Oxford*; S. D. Peyerimhoff, *Bonn*; A. Pines, *Berkeley*; M. Quack, *Zurich*; D. J. Tildesley, *Southampton*; A. Wokaun, *Zurich*.

Editorial Board

M. P. Allen, *Bristol*; L. Andrews, *Charlottesville*; M. N. R. Ashfold, *Bristol*; P. F. Barbara, *Minnesota*; R. J. Bartlett, *Gainesville*; J. Bordé, *Paris*; A. D. Buckingham, *Cambridge*; A. Carrington, *Southampton*; M. S. Child, *Oxford*; P. T. Cummings, *Charlottesville*; P. B. Davies, *Cambridge*; P. G. de Gennes, *Paris*; K. B. Eisenthal, *New York*; R. R. Ernst, *Zurich*; G. Ertl, *Berlin*; P. W. Fowler, *Exeter*; D. Frenkel, *Amsterdam*; G. Graner, *Orsay*; H. Hayashi, *Tokyo*; Ch. Jungen, *Orsay*; M. L. Klein, *Philadelphia*; A. J. Leadbetter, *Grenoble*; R. D. Levine, *Jerusalem*; G. R. Luckhurst, *Southampton*; I. M. Mills, *Reading*; Yu. N. Molin, *Novosibirsk*; R. E. Moss, *Southampton*; K. J. Packer, *Nottingham*; J. G. Powles, *Kent*; B. O. Roos, *Lund*; J. S. Rowlinson, *Oxford*; J. P. Ryckaert, *Brussels*; R. J. Saykally, *Berkeley*; J. P. Simons, *Oxford*; R. E. Smalley, *Houston*; G. A. Somorjai, *Berkeley*; J. Stecki, *Warsaw*; W. A. Steele, *Pennsylvania*; U. E. Steiner, *Konstanz*; R. K. Thomas, *Oxford*; R. Tycko, *Bethesda*; W. Urban, *Bonn*; J. K. G. Watson, *Ottawa*; R. O. Watts, *Seattle*; H. Wennerström, *Lund*; B. Widom, *Cornell*; D. R. Yarkony, *Baltimore*; R. N. Zare, *Stanford*; together with members of the Executive Committee.

Subscription Information

Molecular Physics (*ISSN 0026 8976*) is published 18 times a year by Taylor & Francis Ltd, 4 John Street, London WC1N 2ET, UK.

Annual Subscription 1995 £1112, US $1835.

Second class postage paid at Jamaica, New York 11431. US Postmasters: Send address changes to *Molecular Physics*, Publications Expediting Inc., 200 Meacham Avenue, Elmont, New York 11003. Air freight and mailing in the USA by Publications Expediting Inc., 200 Meacham Avenue, Elmont, New York 11003.

Printed in UK by Burgess Science Press, Rankine Road, Basingstoke, Hampshire RG24 8PR, UK. The paper used in this publication is 'acid free' and conforms to the American National Standards Institute requirements in this respect.

Dollar rates apply to subscribers in all countries except the UK and the Republic of Ireland where the pound sterling price applies. All subscriptions are payable in advance and all rates include postage. Journals are sent by air to the USA, Canada, Mexico, India, Japan and Australasia. Subscriptions are entered on an annual basis, i.e. January to December. Payment may be made by sterling cheque, dollar cheque, international money order, National Giro, or credit card (Amex, Visa, Mastercard/Access).

Orders originating in the following territories should be sent direct to the local distributor. **India:** Universal Subscription Agency Pvt. Ltd, 101–102 Community Centre, Malviya Nagar Extn, Post Bag No. 8, Saket, New Delhi 110017. **Japan:** Kinokuniya Company Ltd, Journal Department, PO Box 55, Chitose, Tokyo 156. **USA, Canada and Mexico:** Taylor & Francis, Inc., 1900 Frost Road, Suite 101, Bristol, Pennsylvania 19007. **UK and all other territories:** Taylor & Francis Ltd, Rankine Road, Basingstoke, Hampshire RG24 8PR.

Advertisements

All enquiries to Taylor & Francis Ltd, Basingstoke (01256) 840366 or Taylor & Francis Inc, Washington, DC (202) 289 2174.

Copyright © 1995 Taylor & Francis Ltd

All rights reserved. Authors are themselves responsible for obtaining permission to reproduce copyright material from other sources and are required to sign a form for agreement of the transfer of copyright. All requests from third parties to reprint material held in copyright by Taylor & Francis must be referred to the author for consent as a condition of the granting by Taylor & Francis of permission for reproduction. No part of this publication may be reproduced, stored in a retrieval system or transmitted in any form, or by any means, electronic, electrostatic, magnetic, mechanical, photocopying, recording or otherwise, without prior permission in writing from the copyright holder.

Authorization to photocopy items for internal or personal use, or the internal or personal use of specific clients, is granted by Taylor & Francis Ltd for libraries and other users registered with the Copyright Clearance Center (CCC) Transactional Reporting Service, provided that the base fee is paid directly to CCC, 27 Congress Street, Salem, Massachusetts 01970, USA. (For fee per article see copyright code shown on the first page of an article in this journal.) This consent does not extend to other kinds of copying, such as copying for general distribution, for advertising, for creating new collective works, or for resale. Fees for past articles are the same as those shown for current articles.

Cumulative Index of Authors
(with titles of papers)

Volumes 61-80 (1987-1993)

AARTS, J.F.M., and CALLOMON, J.H.: Analysis of the $\nu_2'' = 1$ manifold in the $\tilde{A}^2\Sigma^+$-$X^2\Pi$ emission spectrum of N_2O^+, **62**, 637

ABASCAL, J.L.F., *see* Lomba, E.

ABASCAL, J.L.F., and BRESME, F.: Monte Carlo simulation of the equation of state of hard tetrahedral molecules, **76**, 1411

ABBOUTI TEMSAMANI, M., VANDER AUWERA, J., and HERMAN, M.: The absorption spectrum of C_2HD between 9000 and 13 000 cm^{-1}, **79**, 359

ABEN, I., UBACHS, W., VAN DER ZWAN,, G., and HOGERVORST, W.: Polarization effects in resonant four-wave-mixing processes, **76**, 591

ABRAMCZYK, H.: Intramolecular dipole-dipole coupling model for vibrational dephasing in non-rigid molecules. Application for 2-oxo-1,3,2-dioxaphosphorinanes, **64**, 315

ACEVEDO, R., DIAZ, G., LETELIER, J.R., and FLINT, C.D.: Vibronic intensities in the electronic spectra of transition-metal complex ions. Part VII. The $\Gamma_8(^2T_{2g}) \rightarrow \Gamma_8(^2A_{2g})$ electronic transition of the $ReBr_6^{2-}$ ion in Cs_2ZrBr_6, **71**, 1063

ACEVEDO, R., VASQUEZ, S.O.: Vibronic intensities in the electronic spectra of transition metal complex ions. Part IX. Experimental study of the relative vibronic intensities in the $^2E_g \rightarrow {}^4A_{2g}$ transition of the MnF_6^{2-} ion in CS_2SiF_6, **74**, 843

ACEVEDO, R., VASQUEZ, S.O., and FLINT, C.D.: Vibronic intensities in the electronic spectra of transition metal complex ions. Part X. Second order Herzberg-Teller contributions to the vibronic intensity of the $^4A_{2g} \leftrightarrow {}^4T_{1g}$ transition in Mn_6^{2-}, **74**, 853

ACKERMANN, J., and HOGREVE, H.: A CI study of the ground state potential energy surface of He_3^+, **68**, 279

ADACHI, H., *see* Kobayashi, H.

ADAM, C.D., *see* Michopoulos, Y.

ADAMOWICZ, L.: Numerical MCSCF study of the total (electronic and nuclear) parallel polarizability and hyperpolarizability for the H_2, HD and D_2 molecules, **65**, 1047

ADAMOWICZ, L., *see* Slanina, Z.

ADAMS, D.J.: Hard dumbell fluid, g_1 and g_2 from Monte Carlo, **73**, 757

ADAMS, D.J., LUCKHURST, G.R. and PHIPPEN, R.W.: Computer simulation studies of anisotropic systems. XVII. The Gay-Berne model nematogen, **61**, 1575

ADAMS, P., and HENDERSON, J.R.: Molecular dynamics simulations of wetting and drying in LJ models of solid-fluid interfaces in the presence of liquid-vapour coexistence, **73**, 1383

ADYA, A.K., and NEILSON, G.W.. The structure of molten ammonium nitrate by isotopic difference method of neutron diffraction, **69**, 487

ADYA, A.K., and NEILSON, G.W.: Investigation of the structure of an ammonium nitrate-calcium nitrate eutectic melt using isotopic difference methods in neutron diffraction, **71**, 1091

ADYA, A.K., NEILSEN, G.W., OKADA, I., and OKAZAKI, S.: The determination of the radial distribution functions $g_{Li\text{-}Li}(r)$, $g_{Li\text{-}O}(r)$ and $g_{Li\text{-}N}(r)$, in molten lithium nitrate from neutron diffraction, **79**, 1327

ADYA, A.K., TAKAGI, R., KAWAMURA, K., and MIKAMI, M.: Structural determination of molten $NaNO_3$, $NaNO_2$ and their eutectic mixture by molecular dynamics simulation and X-ray diffraction, **62**, 227

ADYA, A.K., and WORMALD, C.J.: First direct observation of orientationally correlated molecules in CO_2(1) by neutron diffraction, **74**, 735

ADYA, A.K., and WORMALD, CJ.: Intra and intermolecular structure in the condensed phases of ethylene, ethane and carbon dioxide by neutron diffraction, **77**, 1217

ADYA, A.K., and WORMALD, C.J.: Excess intermolecular structure and pair correlation functions in liquid mixtures 0.5 CO_2 + 0.5 C_2D_4 and 0.5 CO_2 + 0.5 C_2D_6 by neutron diffractions, **78**, 1075

AGAFONOV, V., *see* André, D.

AGG, P.J., and CLARY, D.C.: Rotationally inelastic rates and Raman Q-branch linewidths for N_2 + N_2, **73**, 317

AGUILAR, A., BIANCO, S., BRUNETTI, B., GONZALEZ, M., and VECCHIOCATTIVI, F.: Total cross-section for the ionization of molecules by thermal-energy collision with metastable neon atoms, **71**, 897

AGUILAR, A., GONZALEZ, M., and POLUYANOV, L.V.: Analytical treatment of the quadratic and nonrelativistic Renner-Teller effect for a triatomic molecule in an electronic state. I. High energy limit, **77**, 193

AGUILAR, A., GONZALEZ, M., and POLUYANOV, L.V.: Analytical treatment of the quadratic and nonrelativistic Renner-Teller effect for a triatomic molecule in a Π electronic state. II. High energy and high angular momentum limit, **77**, 209

AMAHA, A.: *F* matrix connecting points on opposite sides of a parabolic potential well, **78**, 345

AHLRICHS, R., *see* Hill, J.R.

AHLRICHS, R., *see* Kömel, C.

AHLSTRÖM, P., WALLQVIST, A., ENGSTROM, S., and JOHNSSON, B.: A molecular dynamics study of polarizable water, **68**, 563

ALAMICHEL, C., *see* Ben Sari-Zizi, N.

ALAMICHEL, C., *see* Najib, H.

ALAMICHEL, C., *see* Ouahman, M.

ALANKO, S., *see* Antilla, R.

ALANKO, S., *see* Paso, R.

ALANKO, S., *see* Tolonen, A.-M.

ALAVI, A.: Molecular-dynamics simulation of methane adsorbed on MgO: Evidence for Kosterlitz-Thouless transition, **71**, 1173

ALAVI, A., and MCDONALD, I.R.: Molecular-dynamics simulation of argon physisorbed on magnesium oxide, **69**, 703

ALBERT, I.D.L., *see* Ramasesha, S.

ALDEN, R.G., LIN, S.H., XIAOM W.Z., FAIN, B., and ISLAMPOUR, R.: Theory of femtosecond time-resolved infrared adsorption spectroscopy with application to ligand dissociation in haemoglobin, **75**, 1375

ALDERMAN, D.W., *see* Sethi, N.K.

AL-DERZI, A.R. JOHNSTON, R.L., MURRELL, J.N., and RODRIGUEZ-RUIZ, J.A.: Potential energy functions for atomic solids III. Fitting phonon frequencies and elastic constants of diamond structures, **73**, 265

ALEJANDRE, J., *see* Benavides, A.L.

ALEJANDRE, J., *see* De Lonngi, D.A.

ALEJANDRE, J., and CHAPELA, G.A.: Molecular dynamics for discontinuous potentials. III. Compressibility factors and structure of hard polyatomic fluids, **61**, 1119

ALEJANDRE, J., MARTINEZ-CASAS, S.E., and CHAPELA, G.A.: On the calculation of the sphericity factor for fused hard sphere molecules, **65**, 1185

ALEXANDER, J.J., *see* Harris, K.R.

ALEXANDER, J., *see* Rautter, J.

ALEXIEWICZ, W.: Molecular Kerr relaxation theory for liquids in reorienting pulse fields. The case of small inertial effects, **64**, 81

ALIJAH, A., and DUXBURY, G.: Renner-Teller and spin-orbit interactions between the $^1A_1$, $^1B_1$ and $^3B_1$ states of CH_2, **70**, 605

ALIOTTA, F., *see* Maisano, G.

ALIOTTA, F., *see* Magazc, S.

ALIOTTA, F., *see* Majolino, D.

ALLEN, J.M., ASHFORD, M.N.R., STICKLAND, R.J. and WESTERN, C.M.: The $\tilde{B}E''$ state of NH_3 : the Jahn-Teller effect revealed by infrared-optical double resonance, **74**, 49

ALLEN, M.P.: A theoretical study of the Lebwohl-Lasher model in higher dimensions, **68**, 181

ALLEN, M.P., and MASTERS, A.J.: Computer simulation of a twisted nematic liquid crystal, **79**, 277

ALLEN, M.P., and MASTERS, A.J.: Some notes on Einstein relationships, **79**, 425

ALLEN, M.P., *see* Cleaver, D.J.

ALLEN, M.P., *see* De Miguel, E.

ALLEN, M.P., *see* Hess, S.

ALLEN, M.P., *see* Telo da Gama, M.M.

ALLEN, M.P., *see* Wilson, M.R.

ALLNATT, A.R., *see* Aziz, R.A.

ALLNATT, A.R., *see* Dham, A.K.

ALLNATT, A.R., *see* Watanabe, K.

ALMARZA, N.G., *see* Alvarez, M.
ALMARZA, N.G., *see* Encisco, E.
ALMARZA, N.G., ENCISO, E., ALONSO, J., BERMEJO, F.J., and ALVAREZ, M.: Monte Carlo simulations of liquid n-butane, **70**, 485
ALOISI, G., *see* Boudh-Hir, M.-E.
ALONSO, J., *see* Almarza, N.G.
ALONSO, J., *see* Alvarez, M.
ALONSO, J., *see* Bermejo, F.J.
ALONSO, J.A., *see* Cordero, N.A.
ALONSO, J.A., *see* March, N.H.
ALTONA, C., *see*, Diez, E.
ALTONA, C., *see* Krol, M.C.
ALTONA, C., *see* Smits, F.G.
ALVAREZ, M., *see* Almarza, N.G.
ALVAREZ, M., BERMEJO, F.J., CHIEUX, P., ENCISCO, E., GARCIA-HERNANDEZ, M., GARCIA, N., and ALONSO, J.: The equilibrium structure of highly polar molecular liquids. I. SO_2, **66**, 397
ALVAREZ, M., BERMEJO, F.J., HOWELLS, W.S., ENCISO, E., ALMARZA, N.G., and GARCIA-HERNANDEZ, M.: Pulsed neutron diffraction of liquid n-butane, **71**, 865
ALVAREZ-COLLADO, J.R., and BUENKER, R.J.: Theoretical study of the transition probabilities among the three lowest electronic states of the SeS molecule, **64**, 725
AMAHA, A., and KARLSSON, F.: On Connor's connection formula across a potential well, generalized to phase-integral approximations of arbitrary order, **77**, 491
AMANO, T., *see* Nakanaga, T.
AMAR, J.G.: Application of the Gibbs ensemble to the study of fluid-fluid phase equilibrium in a binary mixture of symmetric non-additive hard spheres, **67**, 739
AMAT, G.: Third order determination of the vibrational spectroscopic constants for a tri-atomic linear molecule affected by Fermi resonance, **63**, 639
AMAT, G.: Linear relations between vibrational energy levels of CO_2 and fourth order spectroscopic constants, **73**, 685
AMIOT, C., *see* Bernard A.
AMIOT, C., *see* Fellows, C.E.
AMIOT, C., *see* Gustavsson, T.
AMIOT, C. and VERGES, J.: The Rb_2 $2^1\Sigma_g^+$ electronic state by laser induced fluorescence infrared Fourier transform spectroscopy, **61**, 51
AMORETTI, G., *see* Caciuffo, R.
AMOROS, J., *see* Maeso, M.J.
AMOS, M.D., and JACKSON, G.: BHS theory and computer simulations of linear heteronuclear triatomic hard-sphere molecules, **74**, 191
AMOS, M.D., *see* Sear, R.P.
AMOS, R.D., *see* Jayatilaka, D.
AMOS, R.D., *see* Laming, G.J.
AMOS, R.D., *see* Smith, C.M.
AMOS, R.D., *see* Tozer, D.J.
AMOUREUX, J.P. *see* Decressain, R.
AMREIN, A., *see* Ross, A.J.
AN, C.Z., and FERANCHUK, I.D.: The operator method in the direct and inverse problems of the spectroscopy, **64**, 589
ANDERSSON, O., and ROSS, R.G.: Thermal conductivity, heat capacity and phase diagram of cyclooctanol in liquid, solid and glassy crystal states under high pressure, **71**, 523
ANDERSSON, O., and ROSS, R.G.: Thermal conductivity of (+)- and (±)-camphor at pressures up to 0.5 GPa and temperatures down to 40K, **76**, 433
ANDERSSON, O., ROSS, R.G., and BACKSTROM, G.: Thermal conductivity of crystalline and glassy crystal cyclohexanol under pressure, **66**, 619
ANDERSSON, O., ROSS, R.G., and JEZOWSKI, A.: Chirality and the thermophysical properties of molecular solid phases under pressure: (+)- and (±)-camphor, **70**, 1065
ANDRÉ, D., DWORKIN, A., SWZWARC, H., CÉOLIN, R., AGAFONOV, F., FABRE, C., RASSAT, A., STRAVER, L., BERNIER, P., and ZAHAB, A.: Molecular packing of fullerene C_{60} at room temperature, **76**, 1311
ANDRÉ, D., *see* Jumeau, D.

ADREANI, C., and TAYLOR, A.D.: Density of vibrational states in hydrogen bonded crystals. Potassium dihydrogen phosphate, **68**, 681

ANDREANI, C., MAYERS, J., POSTORINO, P., and RICCI, M.A.: Stretching density of states of the deuterium sites in polycrystalline D_2O, **73**, 737

ANDREANI, C., MERLO, V., RICCI, M.A., and BOLAND, B.C.: Vibrational density of states in polycrystalline sulphuric acid, **66**, 747

ANDREANI, C., MERLO, V., RICCI, M.A. and SOPER, A.K.: Neutron diffraction study of the partial pair correlation functions of liquid hydrogen sulphide, **73**, 407

ANDREANI, C., and PETRILLO, C.: Neutron and X-ray diffraction patterns of aqueous sulphuric acid solutions, **62**, 765

ANDRÉS, J.L., *see* Marti, J.

ANDRESEN, Y., *see* Jäger, W.

ANDREW, E.R., *see* Buszjim N,K,

ANDREW, E.R., JURGA, K., and SZCZESNIAK, E.: Molecular motions and polymorphic properties of solid 2-methyl-2-propaneselenol as studied by N.M.R., **65**, 1421

ANDREW, E.R., and PEPLINKSKA, B.: NMR study of solid cholesterol, **70**, 505

ANDREWS, L., DAVIS, S.R., and HUNT, R.D.: Far infrared spectra of $(HF)_2$ and $(HF)_3$ in solid argon, **77**, 993

ANDRIESSEN, J., DORENBOS, P. and VAN EIJK, C.W.E.: Electronic structure and transition probabilities in pure and Ce^{3+} doped BaF_2, an explorative study, **74**, 535

ANGELON, R., *see* Colligiani, A.

ANGLADA, J., BRUNA, P.J., and PEYERIMHOFF, S.D.: The electronic spectrum of ScH. An MRD-CI study, **66**, 541

ANGLADA, J., BRUNA, P.J., and PEYERIMHOFF, S.D.: Theoretical investigation of the low-lying electronic states of TiH, **69**, 281

ANTTILA, R., ALANKO, S., HORNEMAN, V.-M., and KOIVUSAAR, M.: Ground State Constants A_0 and D_0^K of $^{13}CH_3I$ from perturbation-allowed transitions, **71**, 1433

ANTTILA, R., *see* Graner, G.

ANTTILA, R., HORNEMAN, V.-M. and ALANKO, S.: Ground-state constants A_0 and D_0^K of $^{12}CH_3I$ from perturbation-allowed transitions, **70**, 991

ANTTILA, R., *see* Paso, R.

ANTISIFEROVA, L.I., IVANOVA, A.N., and KULAGINA, T.P.: On the feasibility of molecular motion studies by the electron-electron double resonance method, **61**, 1299

ANTONCHENKO, V. YA., ILYIN, V.V., MAKOVSKY, N.N., and KHRYAPA, V.M.: Short-range order in cylindrical liquid-filled micropores, **65**, 1171

ANTZUTKIN, O.N., *see* Morozov, V.A.

AOIZ, F.J., *see* Verdasco, E.

APPERLEY, D.C., HAIPING, B., and HARRIS, R.K.: Tin-chlorine coupling in magic-angle spinning N.M.R. spectra, **68**, 1277

APPERLEY, D.C., *see* Mortimer, M.

ARCAS, P., *see* Luchuga-Fossat, L.

ARCHER, A.L., and JACKSON, G.: Theory and computer simulations of heteronuclear diatomic hard-sphere molecules (hard dumbbells), **73**, 881

ARCIONI, A., BERTINELLIS, F., TARRONI, R., and ZANNONI, C.: Time resolved fluorescence depolarization in a nematic liquid crystal, **61**, 1161

ARMSPACH, J.P., *see* Grucker, D.

AROUI, H., BROQUIER, M., CHEVALIER, M., PICARD, A., and BILLING, G.D.: Temperature effects on collision cross sections between some rovibrational states of ammonia gas perturbed by hydrogen and helium, **74**, 897

ASHFORD, M.N.R., *see* Allen, J.M.

ASHFORD, M.N.R., and PRINCE, J.D.: Third harmonic generation in molecular gases, **73**, 297

ASHFOLD, M.N.R., STICKLAND, R.J., and TUTCHER, B.: Multiphoton ionization spectroscopy of phosphine, **65**, 1171

ASHFOLD, M.N.R., TUTCHER, B., and WESTERN, C.M.: Rydberg states of the SH(SD) radical revealed by multiphoton ionization spectroscopy, **66**, 981

ASHIDA, J., *see* Nakai, T.

ÅSTRAND, P.-O., and KARLSTRÖM, G.: Local polarizability calculations with localized orbitals in the uncoupled Hartree-Fock approximation, **77**. 143

ATAMNY, F., BLöCKER, J., DÜBOTZKY, A., KURT, H., LOOSE, g., MAHDI, W., TIMPE, O., and SCHLÖGL, R.: Surface chemistry of carbon. Activation of molecular oxygen, **76**, 851

ATHERTON, N.M., and BLACKFORD, R.D.S.: Single crystal proton ENDOR of γ-irradiated ammonium paramolybate at 15K. The location of the paramagnetic centre in the $\{MO_7O_{24}\}^{6-}$ ion, **61**, 443

ATKINSON, R.A., CLIFFORD, P., and GREEN, N.J.B.: Correlation effects in simple liquids, **72**, 363

ATTAL-TRÉTOUT, B., *see* Bervas, H.

ATTAL-TRÉTOUT, B., BERLEMONT, P., and TARAN, J.P.: Invited Article. Three-colour CARS spectroscopy of the OH radical at triple resonance, **70**, 1

ATTAL-TRÉTOUT, B., MONOT, P., and MULLER-DETHLEFS, K.: Theory of rotational line strengths in coherent anti-Stokes Raman spectroscopy, **73**, 1257

ATTARD, G.S., see Jones, P.

ATTARD, P.: An improved Kirkwood superposition approximation for three atoms in rolling contact, **74**, 547

ATTARD, P.: Expansion moments for the local field distribution that involve the three-particle distribution function, **75**, 975

ATTARD, P., and MOULE, G.A.: A force-balance Monte Carlo simulation of the surface tension of a hard-sphere fluid, **78**, 943

AUGSPURGER, J.D., and DYKSTRA, C.E.: Magnetic and electrical properties of benzene, **76**, 229

AUGSPURGER, J.D., and DYKSTRA, C.E.: Isotropic and anisotropic proton chemical shielding surface of water, **80**, 117

AURIEMMA, F., *see* Depner, M.

AUSSENEGG, F.R., *see* Kümmerlen, J.

AUSTIN, D, *see* Lawley, K.P.

AVENT, A.G., *see* Celebre, G.

AYRES, J.S., *see* Joshi, Y.P.

AYLLÓN, A.G., SANTAMARÍA, J., MILLER, S., and TENNYSON, J.: Calculated spectra for the N_2-Ar van der Waals complex, **71**, 1043

AZIZ, R.A., *see* Dhamn, A.K.

AZIZ, R.A., MCCOURT, F.R.W., and WONG, C.C.K.: A new determination of the ground state interatomic potential for He_2, **61**, 1487

AZIZ, R.A., SLAMAN, M.J., KOIDE, A., ALLNATT, A.R., and MEATH, W.J.: Exchange-Coulomb potential energy curves for He-He, and related physical properties, **7**, 321

BÄCKSTRÖM, G., *see* Andersson, O.

BÄCKSTRÖM, G., *see* Fransson, A.

BACHEM, E., *see* Lipus, K.

BACHEM, E., *see* Nelis, Th.

BACHEM, E., *see* Towle, J.P.

BACHEM, E., URBAN, W., and NELIS, T.: Direct observation of the transitions $^2\Delta_{5/2}$, $v = 0 \rightarrow {}^2\Pi_{3/2}$, $v = 0$ and $^2\Delta_{5/2}$, $v = 0 \rightarrow {}^2\Delta_{3/2}$ $v = 1$ of the NiH radical by Faraday LMR, employing a CO overtone laser, **73**, 1031

BACHEM, E., *see* Zimmermann, W.

BACKSAY, G.B.: Hydrogen bonded complexes of HCl with CO, C_2H_2, C_2H_4, PH_3, H_2S, HCN, H_2O and NH_3. Correlated quantum chemical calculations of geometries, energetics, vibrational frequencies and ^{35}Cl quadrupole coupling constants, **77**, 61

BACKSAY, G.B., *see* Cummings, P.L.

BACKSAY, G.B., *see* Wong, A.T.

BADER, R.F.W., *see* Carroll, M.T.

BADER, R.F.W., KEITH, T.A., GOUGH, K.M., and LAIDIG, K.E.: Properties of atoms in molecules: additivity and transferability of group polarizabilities, **75**, 1167

BADIALI, J.P., *see* Zhang, Q.

BADIRKHAN, Z., PASTORE, G., and TOSI, M.P.: Charged hard spheres in a uniform neutralizing background: the role of thermodynamic self consistence, **74**, 1089

BAER, M., and ENGLMAN, R.: A study of the diabatic electronic representation within the Born-Oppenheimer approximation, **75**, 293

BAER, S.: Hyperpolarizability dependent dispersion forces and absorption spectra in simple liquids, **65**, 263

BAER, S., *see* Gutman, L.

BAFILE, U., ULIVI, L., ZOPPI, M., and PESTELLI, S.: The third virial coefficient of depolarized-light-scattering spectral moments for moderately quantum systems, **79**, 179
BAGGOTT, J.E.: The relationship between the models of anharmonically and harmonically coupled anharmonic oscillators, **62**, 1019
BAGGOTT, J.E.: Normal modes and local modes in H_2X: beyond the x, K relations, **65**, 739
BAGGOTT, J.E., LAW, D., and MILLS, I.M.: C-H and C-D interbond coupling in $CHDCl_2$, **61**, 1309
BAGGOTT, J.E., NEWNHAM, D.A., DUNCAN, J.L., MCKEAN, D.C., and BROWN, A.: C-H and C-D interbond coupling in CHD_2Cl, **70**, 715
BAIKER, A., *see* Walther, K.L.
BAJAJ, P.N., *see* Talukdar, R.
BAILLEUL, S., and PORCHER, P.: Simulation of energy levels schemes and of some magnetic properties of divalent copper in tetragonal or pseudo tetragonal symmetries, **66**, 605
BAKER, J., *see* Barnes, M.
BAKHRAKH, V.L., *see* Vetchinkin, S.I.
BAKKER, A.F., *see* Nijmeijer, M.J.P.
BAKÓ, I., *see* Pálinkás, G.
BALASUBRAMANIAN, K., *see* Hongxing Zhang
BALASUBRAMANIAN, K., *see* Wang, J.Z.
BALASUBRAMANIAN, K.: Characterization of Hadamard matrices, **78**, 1309
BALASUBRAMANIAN, K.: Nuclear spin multiplets for five $^{13}C_{78}$ fullerene isomers, **80**, 655
BALFOUR, W.J., LAUNILA, O., and KLYNNING, L.: Fourier transform spectroscopy of MnH and MnD. Rotational analyses of the 846 nm and 1060 nm systems, **69**, 443
BALDO, M., GRASSI, A., and PERLY, B.: Angular correlation function for N.M.R. relaxation times. A general description for molecules with multiple internal rotations, **64**, 51
BALIBANU, F., *see* Ursu, I.
BALL, P.C., *see* Smalley, M.V.
BALL, P.C., and EVANS, R.: The density profile of a confined fluid. Comparison of density functional theory and simulation, **63**, 159
BANICHEVICH, A., KLOTZ, R., and PEYERIMHOFF, S.D.: Predissociation of the ions HBr^+ and DBr^+, **75**, 173
BANKS, M.R. *see* Jones, A.C.
BALUCANI, U.: Shear viscosity in monatomic liquids: a simple mode-coupling approach, **71**, 123
BAOQI MENG, BRUNA, P.J., and WRIGHT, J.S.: Stability of highly excited electronic states of Be_2^+, **79**, 1305
BARAM, A., and ROWLINSON, J.S.: Studies of the Gaussian model I. The one-component system, **74**, 707
BARAM, A., MADDOX, M.W., and ROWLINSON, J.S.: Studies of the Gaussian model. II. The two-component system, **76**, 1093
BARAM, A., MADDOX, M.W., and ROWLINSON, J.S.: Studies on the Gaussian model. III. The three-component system, **79**, 589
BARANYAI, A., *see* Evans, D.J.
BARANYAI, A., and EVANS, D.J.: New algorithm for constrained molecular-dynamics simulation of liquid benzene and naphthalene, **70**, 53
BARANYAI, A., and EVANS, D.J.: NEMD investigation of the rheology of oblate molecules: shear flow in liquid benzene, **71**, 835
BARANYAI, A., and EVANS, D.J.: Calculation of equilibrium entropy differences from non-equilibrium molecular dynamics simulations, **72**, 229
BARANYAI, A., and EVANS, D.J.: Comments on thermodynamic integration methods for the determination of non-equilibrium entropy, **74**, 353
BARANYAI, A., and WELBERRY, T.R.: Molecular dynamics simulation of solid biphenyl, **73**, 1317
BARANYAI, A., and WELBERRY, T.R.: Molecular dynamics simulation study of solid polyphenyls: Structures determined by the interplay between intra- and intermolecular forces, **75**, 867
BARANYAI, Y., *see* Evans, D.J.
BARBIERI, R.S., and BONHAM, R.A.: The dielectric dispersion surface for the nitrogen molecule in the gas phase, **77**, 1055
BARENDSWAARD, W., VAN TOL, J., WEBER, R.T., and VAN DER WAALS, J.H.: The luminescent triplet state of the $Ba_3(VO_4)_2$ crystal. I. Determination of the spin hamiltonian by E.P.R. at 1.2K, **67**, 651
BARKER, G.C., *see* Grimson, M.J.
BARKER, G.C., and GRIMSON, M.J.: A model suspension of deformable particles, **62**, 269

BARKER, G.C., and GRIMSON, M.J.: Random sequential adsorption of lattice shapes onto a square lattice, **63**, 145

BARKER, J.A.: Surface tension and atomic interactions in simple liquids. Argon, krypton and xenon, **80**, 815

BARNARD, S.A., FORD, M.J., COOPER, D.L., GERRATT, J., and RAIMONDI, M.: Calculation of potential energy curves for electron capture by C^{3+} from neutral lithium using spin-coupled VB theory, **61**, 1193

BARNES, L.A., CHANDLER, G.S., and FIGGIS, B.N.: Orbital magnetization in $CoCl_4^{2-}$ and Co(phthalocyanine) from polarized neutron diffraction, **68**, 711

BARNES, M., BAKER, J., DYKE, J.M., FEHER, M., and MORRIS, A.: An investigation of the $SO(X^3\Sigma^-)$ molecule by multiphoton ionization spectroscopy, **74**, 689

BARNICKEL, P., and WOKAUN, A.: Silver coated latex spheres. Optical absorption spectra and surface enhanced Raman scattering, **67**, 1355

BARNICKEL, P., and WOKAUN, A.: Synthesis of metal colloids in inverse microemulsions, **69**, 1

BARRAT, J.L., HANSEN, J.P., and PASTORE, G.: On the equilibrium structure of dense fluids. Triplet correlations, integral equations and freezing, **63**, 747

BARRAT, J.-L., and MCDONALD, I.R.: The role of molecular flexibility in simulations of water, **70**, 535

BARREAU, A., CHAVE, A., DUMON, B., THIBEAU, M., and LADANYI, B.: Effects of intermolecular interactions on depolarized Rayleigh scattering intensities of fluids of linear molecules. A computer simulation study, **67**, 1241

BARREAU, A., *see* Ladanyi, B.M.

BARRON, L.D., *see* Escribano, J.R.

BARRON, L.D., *see* Hecht, L.

BARRON, L.D., and JOHNSTON, C.J.: Discrimination in the dispersion interaction between odd-electron chiral molecules, **62**, 987

BARRON, L.D., and POLAVARAPU, P.L.: Raman optical activity in ring deformations of methyloxirane, methylthirane and trans-2,3-dimethyloxirane, **65**, 659

BARROW, R.F., *see* Bernard, A.

BARROW, R.F., *see* Effantin, C.

BARROW, R.F., HOWARD, B.J., BERNARD, A., and EFFANTIN, C.: The $A'\,^2\Delta$-$X^2\Sigma^+$ transition in BaH, **72**, 971

BARTELL, L.S., *see* Dove, M.T.

BARTELL, L.S., *see* Powell, B.M.

BARTELL, L.S., and POWELL, B.M.: Proposed model for disorder in the warmest crystalline phase of C_4F_8, **67**, 861

BARTELL, L.S., and POWELL, B.M.: Crystal structures of the low temperature phases of TeF_6, **75**, 689

BARTHELAT, J.C., *see* Bouteiller, Y.

BARTLEET, J.M., DENNING, R.G., MORRISSON, I.D.: The electronic structure of actinyl ions. Part IX. The electronic spectroscopy of $(PPh_4)UOCl_5$, **75**, 601

BARTLETT, P., and HOWARD, B.J.: The rotational-vibrational spectrum of symmetric non-rigid triatomics in hyperspherical coordinates: the H_3^+ molecule, **70**, 1001

BASILE, A.G., GRAY, C.G., NICKEL, B.G., and POLL, J.D.: Lineshapes in collision-induced absorption. Classical, quantum and semiclassical calculations for exactly solvable models, **66**, 961

BASILEVSKY, M.V., and CHUDINOV, G.E.: New formulation of adiabatic theory of electron transfer in polar media, **65**, 1121

BASILEVSKY, M.V., and CHUDINOV, G.E.: Kinetics of outersphere electron transfer in non-Debye solvents with two characteristic relaxation periods, **71**, 461

BASTIAN, E.W., HUIS, L., and MACLEAN, C.: Study of angular correlation by N.M.R. of magnetically aligned molecules, **67**, 615

BATCHELOR, S.N., MCLAUCHLAN, K.A., and SHKROB, I.A.: Reaction yield detected magnetic resonance in exciplex systems. I. B_0 and B_1 spectra, **75**, 501

BATCHELOR, S.N., MCLAUCHLAN, K.A., and SHKROB, I.A.: Reaction yield detected magnetic resonance in exciplex systems. II. Time resolved and pulse studies, **75**, 531

BATCHELOR, S.N., MCLAUCHLAN, K.A., and SHKROB, I.A.: Reaction yield detected magnetic resonance and magnetic field effect studies of radical pairs containing electronically excited organic radicals, **77**, 75

BAUDER, A., *see* Jans-Bürli, S.

BAUERLE, P., *see* Sacriciftci, N.S.

BAUMANN, W., *see* Rodrigues, S.V.

BAUS, M., *see* Dupont, G.
BAUS, M., *see* Wu,G .
BAUSENWEIN, T., BERTAGNOLLI, H., GUTWERK, D., TÖDHEIDE, K., and CHIEUX, P.: The structure of fluid carbon dioxide by neutron diffraction at high pressure and by RISM calculations, **76**, 127
BEAMSON, G., and BRIGGS, D.: High resolution monochromated X-ray photoelectron spectroscopy of organic polymers. A comparison between solid state data for organic polymers and gas phase data for small molecules, **76**, 919
BEARPARK, M.J., HANDY, N.C., PALMIERI, P., and TARRONI, R.: Spin-orbit interactions from self consistent field wavefunctions, **80**, 479
BEATTIE, I.R., *see* Burghardt, I.
BEATTIE, I.R., JONES, P.J., and YOUNG, N.A.: Nickel dichloride: A nonlinear molecule in a nitrogen matrix? Implications for structure determinations in cryogenic matrices, **72**, 1309
BECKMANN, P.A., HATHORN, R.M., and MALLORY, F.B.: Proton Zeeman relaxation and intramolecular reorientation in solid *t*-butylbenzene, **69**, 411
BEDANOV, V.M.: Computer simulation of cluster decay, **69**, 1011
BEDEAUX, D., *see* Blokhuis, E.M.
BÉE, M., *see* Carpentier, L.
BÉE, M., *see* Giroud-Godquin, A.M.
BELAFHAL, A., *see* Chapuisat, X.
BELCHIOR, J.C., MURRELL, J.N., and BOSANAC, S.C.: The hardness factor in rotational inelastic scattering, **77**, 727
BELL, A.J., and FREY, J.G.: Raman emission from the photolysis of NOCl at 266 nm, **69**, 943
BELL, A.J., PARDON, P.R., and FREY, J.G.: Raman spectra of NOCl and Cl_2. Photo-dissociation dynamics, **67**, 465
BELLEMANS, A., *see* Depaepe, J.M.
BELLEMANS, A., *see* Maréchal, G.
BELLISSENT-FUNEL, M.-C., BUONTEMPO, U., PETRILLO, C., and RICCI, F.P.: Orientational correlation in liquid CO: neutron-diffraction measurements, **71**, 239
BELLISSENT-FUNEL, M.-C., BUONTMPO, U., PETRILLO, C., and RICCI, F.P.: Structure of liquid chlorine from neutron-diffraction measurements, **71**, 253
BELLISSENT-FUNEL, M.-C., BUONTEMPO, U., PETRILLO, C., and RICCI, F.P.: Structure factor measurements of liquid Cl_2 at high temperature, **74**, 1209
BELLISSENT-FUNEL, M.-C., *see* Farman, H.
BELLISSENT-FUNEL, M.-C., *see* Powell, D.H.
BELORIZKY, E., FRIES, P.H., GOJON, E., and LATOUR, J.-M.: An efficient diagonalization method for fitting the exchange constants in a spin cluster from susceptibility data. Application to a pentacopper(II) complex, **61**, 661
BELORIZKY., E., and REY, P.: Interpretation of the magnetic behaviour of an hexakis manganese (II)-nitroxide oligonuclear complex, **75**, 563
BELTON, P.S., *see* Hills, B.P.
BELTON, P.S., and HILLS, B.P.: The effects of diffusive exchange in heterogeneous systems on N.M.R. line shapes and relaxation processes, **61**, 999
BELTON, P.S., and HILLS, B.P.: The effects of exchange and interfacial reaction in two-phase systems on N.M.R. lineshapes and relaxation processes, **65**, 313
BELTON, P.S., HILLS, B.P., and RAIMBAUD, E.R.: The effects of morphology and exchange on proton N.M.R. relaxation in agarose gels, **63**, 825
BELTON, P.S., RING, S.G., BOTHAM, R.L., and HILLS, B.P.: Multinuclear NMR studies of water in solutions of simple carbohydrates. II. Oxygen-17 relaxation, **72**, 1123
BEN-AMOTZ, D., *see* De Souza, L.E.S.
BENASSI, P., MAZZACURATI, V., NARDONE, M., RICCI, M.A., RUOCCO, G., DE SANTIS, A., FRATTINI, R., and SAMPOLI, M.: Raman spectra of water in the translational and librational region. II. Temperature evolution of the isotropic component, **62**, 1467
BENAVIDES, A.L., ALEJANDRE, J., and DEL RIO, F.: Properties of the square-well fluid of variable width. IV. Molecular dynamics test of the van der Waals and long-range approximations, **74**, 321
BENAVIDES, A.H., and DEL RIO, F.: Properties of the square-well fluid of variable width. III. Long-range expansion, **68**, 983
BENAVIDES, A.L., *see* Del Rio, F.
BENCIVENNI, L., *see* Ramondo, F.R.
BENETIS, N., *see* Westlund, P.-O.

BENGTSSON, L.A., STEGEMANN, H., HOLMBERG, B., and FULLBIER, H.: The structure of room temperature molten polyiodides, **73**, 283

BÉNIÈRE, F.M., FUCHS, A.H., DE FERAUDY, M.-F., and TORCHET, G.: The hexagonal phase of sulfur hexafluoride by molecular dynamics simulation of free clusters, **76**, 1071

BENNETT, B., and RAYNES, W.T.: Temperature dependence of the carbon-13 proton spin-spin coupling constant in gaseous methane. Theory and experiment, **61**, 1423

BENOIT, A.-M.: Effet Kerr et polarisabilites moleculaires du bromotrifluoromethane, **65**, 487

BERRONDO, M., and LARSEN, S.Y.: Two-body density of states of hard spheres at high energies, **65**, 345

BENSARI-ZIZI, N., *see* Najib, H.

BEN SARI-ZIZI, N., and ALAMICHEL, C.: The perpendicular $\upsilon_4^{\pm 1} + \upsilon_6^{\pm 1}$ component of the rovibrational $\upsilon_4 + \upsilon_6$ band of $CH_3\ ^{79}Br$, studied in a high resolution FTIR spectrum from 3870 to 4100 cm^{-1}, **80**, 515

BERBLINGER, M., and SCHLIER, C.: Classical radiation spectra of long-lived H_3^+-complexes, **63**, 779

BERENGOL'TS, T.S., *see* Tsukerblat, B.S.

BERENDSEN, H.J.C., *see* Juffer, A.H.

BERG, L.-E., ROYEN, P., and WEIJNITZ, P.: Lifetime measurements of CaCl, CaBr and SrCl. Radiative lifetimes of the $B^2\Sigma^+$ states, **69**, 385

BERG, L.-E., OLSSON, T., CHANTELOUP, J.-C., HISHIKAWA, A., and ROYEN, P.: Lifetime measurements of excited molecular states using a Ti:sapphire laser. Radiative lifetimes of the $A^2\Pi$, $B^2\Sigma$ and $C^2\Pi$ states of BaF, **79**, 721

BERGER, H., *see* Lavorel, B.

BERGNER, A., DOLG, M., KÜCHLE, W., STOLL, H., and PREUSS, H.: *Ab initio* energy-adjusted pseudopotentials for elements of groups 13-17, **80**, 1431

BERLEMONT, P., *see* Attal-Trétout, B.

BERMEJO, F.J., *see* Almarza, N.G.

BERMEJO, F.J., *see* Alvarez, M.

BERMEJO, F.J., *see* Chahid, A.

BERMEJO, F.J., *see* Criado, A.

BERMEJO, F.J., ENCISCO, E., ALONSO, J., GARCIA, N., and HOWELLS, W.S.: How well do we know the structure of simple molecular liquids? CCl_4 revisited, **64**, 1169

BERMEJO, F.J., *see* Enciso, E.

BERMEJO, F.J., *see* Esteban, A.L.

BERMEJO, F., *see* Guilleme, J.

BERMEL, W., *see* Ernst, M.

BERNARD, A., *see* Barrow, R.F.

BERNARD, A., *see* Effantin, C.

BERNARD, A., EFFANTIN, C., D'INCAN, J., AMIOT, C., and VERGÈS, J.: On the 3d Rydberg states of the NO molecule, **73**, 221

BERNARD, A., EFFANTIN, C., D'INCAN, J., FABRE, G., EL HACHIMI, A., STRINGAT, R., VERGÈS, J., and BARROW, R.F.: The *5d* complex of barium hydride; BaH and BaD, **62**, 797

BERNARD, A., EFFANTIN, C., D'INCAN, J., FABRE, G., STRINGAT, R., and BARROW, R.F.: The *5d* states of barium hydride; BaH and BaD, **67**, 1

BERNARD, A., EFFANTIN, C., D'INCAN, J., VERGÈS, J., and BARROW, R.F.: Studies of the electronic states of the BaF molecule. Part II : The 5d(v = 0, 1, 2) states, **70**, 747

BERNARDI, F., BOTTONI, A., and ROBB, M.A.: An MCSCF/MP2 study of methylene insertion-abstraction reactions with C-H and C-Cl bonds, **77**, 51

BERNATH, P.F., *see* Douay, M.

BERNATH, P.F., *see* Rogers, S.

BERNATH, P.F., *see* Walker, K.A.

BERNHARD, T., ZIMMERMAN, H., and HAEBERLEN, U.: The orientations and dynamics of ethanol guest molecules in the clathrate of Dianin's compound. A ^{2}H-nuclear magnetic resonance single crystal study, **77**, 1123

BERNIER, P., *see* André, D.

BERRONDO, M., and LARSEN, S.Y.: Two-body density of states of hard spheres at high energies, **65**, 345

BERRONDO, M., *see* Récamir, J.

BERRY, M.T., KIRBY, A.F., and RICHARDSON, F.S.: Vibronic transitions in the excitation and emission spectra of hexakis(antipyrine)europium(III) tri-iodide and tri-perchlorate crystals, **66**, 723

BERRY, M.T., and RICHARDSON, F.S.: Optical spectra and crystal-field analyses of samarium in the centrosymmetric hexakis(antipyrine)samarium(III) tri-iodide and tri-perchlorate systems, **66**, 703

BERRY R.S., *see* Ojha, P.C.

BERSUKER, G.I., CHIBOTARU, L.F., POLINGER, V.Z., and SOLONENKO, A.O.: Effects of vibrational intercentre interaction in a trigonal two-centre system with twofold electronic degeneracy at each centre. Part I. Theoretical investigation, **70**, 1031

BERSUKER, G.I., CHIBOTARU, L.F., POLINGER, V.Z., and SOLONENKO, A.O.: Effects of vibrational intercentre interaction in a trigonal two-centre system with twofold electronic degeneracy at each centre. Part II. Experimental manifestations, **70**, 1045

BERTAGNOLLI, H., *see* Mager, T.

BERTAGNOLLI, H., *see* Bausenwein, T.

BERTHIER, G., *see* de Brouckére, G.

BERTINELLI, F., *see* Arcioni, A.

BERTOLINI, D., TANI, A., and VALLAURI, R.: Collective motion and interparticle correlations in liquid water. A molecular dynamics simulation, **73**, 69

BERTOLINI, D., and TANI, A.: Librational dynamics of water in terms of angular velocity correlation functions and orientational structure, **75**, 1047

BERTOLINI, D., and TANI, A.: The frequency and wavelength dependent dielectric permittivity of water, **75**, 1065

BERTRAN, J., *see* Marti, J.

BERVAS, H., LE BOITEUX, S., LABRUNIE, L., and ATTAL-TRÉTOUT, B.: Rotational line strengths in degenerate four wave mixing, **79**, 911

BESNARD, M., *see* Cabaço, M.I.

BESNARD, M., FOUASSIER, M., LASSEGUES, J.C. DIANOUX, A.J., and PETRY, W.: Incoherent neutron scattering study of the pseudorotational and diffusive motions of cyclopentane in condensed state, **73**, 1059

BHANUPRAKASH, K., HIRSCH, G., and BUENKER, R.J.: Dipole-forbidden transitions in Se_2: *ab initio* calculations of the radiative lifetimes of the $a'^1\Delta_g$ and $b'^1\Sigma_g^+$, **72**, 1187

BHANUPRAKASH, K., *see* Perić

BHAT, H.L., *see* Murthy, K.

BHAT, S.V., *see* Murthy, K.

BHETHANABOTLA, V.R., and STEELE, W.A.: Triplet correlation functions for fluids of non-spherical molecules, **68**, 659

BHUTYAN, L.B., *see* Outhwaite, C.W.

BIANCO, S., *see* Aguilar, A.

BIBEN, T., and HANSEN, J.-P.: Localized density profiles in binary colloidal suspensions, **80**, 853

BICKEL, G.A., *see* Meenakshi, A.

BILLING, G.D., *see* Aroui, H.

BILLING, G., *see* Broquier, M.

BILLY, N., GIRARD, G., GOUÉDARD, G., and VIGUE, J.: Coherent saturation effects in laser induced fluorescence detection of reaction products. Theory and experiment, **61**, 65

BILLY, N., *see* Gouédard

BILLY, N., *see* Zalicki, P.

BINBREK, O.S., *see* Torrie, B.H.

BIRNBAUM, G., and BORYSOW, A.: On the problem of detailed balance and model lineshapes in collision-induced rotovibrational bands: H_2-H_2 and H_2-He, **73**, 57

BIRNBAUM, G., *see* Brown, M.S.

BIRNBAUM, G., *see* Dore, P.

BIRNBAUM, G., *see* Guillot, B.

BISANTI, P., *see* Andreani, C.

BISCARINI, F., *see* Chiccoli, C.

BISCARINI, F. ZANNONI, C., CHICCOLI, C., and PASINI, P.: Head-tail asymmetry and ferro-electricity in uniaxial liquid crystals. Model calculations, **73**, 439

BISHOP, D.M., *see* Cybulski, S.M.

BISHOP, D.M., and CYBULSKI, S.M.: An analysis of the Verdet constant, **71**, 667

BISHOP, D.M., and CYBULSKI, S.M.: Calculations of magnetic properties. III. Nuclear shielding polarizabilities for H_2, N_2, HF, and CO, **80**, 199

BISHOP, D.M., and CYBULSKI, S.M.: Electron-correlated calculations of the nuclear shielding constants and shielding polarizabilities for H_2, N_2, HF, and CO, **80**, 209

BISHOP, D.M., and LAM, B.: An *ab initio* study of third-order non-linear optical properties of H_2^+, **62**, 721

BISHOP, D.M., and LAM, B.: An analysis of the interaction between a distant point charge and H_2^+, **65**, 679

BISHOP, D.M., and PIPIN, J.: Temperature-dependence of the dynamic dipole polarizability of H_2, **72**, 961

BISSONETTE, E.C., and MCCOURT, F.R.W.: A study of the single-moment, two-moment and multilevel descriptions of depolarized Rayleigh light scattering in molecular gases, **70**, 65

BISWAS, S.N., *see* Sun, T.F.

BITTNER, D.N., *see* Willey, D.R.

BIZOT, P., ECHARGUI, M.A., MARSAULT, J.P., and MARSAULT-HERAIL, F.: Vibrational dephasing in H_2 and HD dissolved in liquid and hypercritical argon, **79**, 489

BLACK, J.F., HASSELBRINK, E., WALDECK, J.R., and ZARE, R.N.: Photofragment orientation as a probe of near-threshold non-adiabatic phenomena in the photodissociation of ICN, **71**, 1143

BLACKFORD, R.D.S., *see* Atherton, N.M.

BLANQUET, G., *see* Dang-Nhu, M.

BLÖCKER, J., *see* Atamny, F.

BLUM, L., *see* Chan, K.-Y

BLÜMICH, B., *see* Günther, E.

BLÜMICH, B., *see* Paff, J.

BOCK, C.W., *see* Caminati, W.

BODDENBERG, B., *see* Grundke, V.

BODDENBERG, B., and NEUE, G.: An N.M.R. study of an *n*-butane film on graphite. I. ^2H relaxation of the 2D fluid state, **67**, 385

BODDENBERG, B., and NIEPMANN, R.: Lateral interactions between ammonia molecules adsorbed on titania (rutile) studied by ^2H NMR, **79**, 405

BODDENBERG, B., *see* Neue, G.

BODEN, N., *see* Kahol, P.K.

BODENHAUSEN, G., *see* Burghardt, I.

BODENHAUSEN, G., *see* Wimperis, S.

BOGEY, M., DAVIES, P.B., DEMUYNCK, C., DESTOMBES, J.L., and SEARS, T.J.: The microwave spectrum of the FO_2 radical, **67**, 1033

BOGEY, M., DEMUYNCK, C., and DESTOMBES, J.L.: Submillimetre wave spectra of the ^{13}C monosubstituted forms of CCH. Determination of the substitution structure, **66**, 955

BOGDAN, M., *see* Ursu, I.

BOHLE, W., *see* Havenith, M.

BOHLE, W., *see* Nelis, Th.

BÖHM, M.C., and SCHÜTT, J.: On the location of π electrons in linear and cyclic hydrocarbons, **72**, 1159

BÖHM, M.C., and SCHÜTT, J.: Many-particle effects in the bond length alternation of alternant hydrocarbons, **75**, 961

BÖHM, M.C., SCHULTE, J., and UTRERA, L.: Material properties of one-dimensional systems studied by path-integral quantum Monte Carlo simulations and an analytical many-body model, **79**, 1239

BOHN, M., *see* Fischer, J.

BOHN, M., FISCHER, J., and HAILE, J.M.: Effect of molecular elongation on the quadrupolar free energy in diatomic fluids, **65**, 797

BOHN, M., LUSTIG, R., FISCHER, J., and KOHLER, F.: Thermodynamic perturbation theory for mixtures of spherical and tetrahedral molecules, **64**, 595

BOLAND, B.C., *see* Andreani, C.

BONDARENKO, G.V., and GORBATY, Y.E.: An infrared study of water vapour in the temperature range 573-723K. Dimerization enthalpy and absorption intensities for monomer and dimer, **74**, 639

BONDYBEY, V.E., *see* Hsu, Y.-C.

BONE, R.G.A., ROWLANDS, T.W., HANDY, N.C., and STONE, A.J.: Transition states from molecular symmetry groups: Analysis of non-rigid acetylene trimer, **72**, 33

BONHAM, R.A., *see* Barbieri R.S.

BONZEL, H.P., *see* Knauff, O.

BOON, T.D., *see* Dodd, L.R.

BOOTH, A.D., and PACKER, K.J.: Magnetic spin lattice relaxation in the presence of spin-diffusion. The one-dimensional, two-region system, **62**, 811

BOPP, P., *see* Pálinkás, G.

BOQUILLON, J.P., *see* Ouazzany, Y.

BORDÉ, J., *see* Palma,

BORGMANN, D., *see* Ganzmann, I.

BORGMANN, D., *see* Heras, J.M.
BORYSOW, A., *see* Birnbaum, G.
BORYSOW, J., FROMMHOLD, L., and KETO, J.W.: The third-order Raman spectrum of argon pairs, **66**, 221
BOSANAC, S.D., *see* Belchoir, J.C.
BOSI, P., *see* Felici, R.
BOTHAM, R.L., *see* Belton, P.S.
BOTTONI, A., *see* Bernadi, F.
BOTSCHWINA, P., HORN, M., SEEGER, S., and FLÜGGE, J.: Equilibrium geometry of HC_3N, **78**, 191
BOUBLÍK, T.: Equation of state of planar hard dumbells, **63**, 685
BOUBLÍK, T.: Convex molecule perturbation theory for the gaussian overlap system. **65**, 209
BOUBLÍK, T.: The gaussian overlap model again, **67**, 1327
BOUBLÍK, T.: Equation of state of linear fused hard-sphere models, **68**, 191
BOUBLÍK, T.: Perturbation theory of pure quadrupolar hard Gaussian overlap fluids, **69**, 497
BOUBLÍK, T.: Equilibrium behaviour of quadrupolar Kihara molecule fluids, **73**, 417
BOUBLÍK, T.: Perturbation theory of polar nonspherical molecule fluids, **76**, 327
BOUBLÍK, T.: Perburbation theory of the quadrupolar Kihara fluid, **77**, 983
BOUBLÍK, T., and DÍAZ PEÑA, M.: The equation of state of hard Gaussian-overlap fluids, **70**, 1115
BOUBLÍK, T., *see* Muller, A.
BOUBLÍK, T., *see* Triska, B.
BOUBLÍK, T., VEGA, C., LAGO, S., and DÍAZ PEÑA, M.: Quadrupolar hard Gaussian-overlap fluid, **71**, 1193
BOUCHIR, M., PERROT, M., and LEICKNAM, J.-CL.: Raman study of rotational motions of hydrogen sulphide in the liquid state, **62**, 679
BOUDH-HIR, M.-E.: New developments for inhomogeneous fluids, **63**, 939
BOUDH-HIR, M.-E.: A self-consistent treatment of a fluid in an external potential, **64**, 437
BOUDH-HIR, M.-E., ALOISI, G., and GUIDELLI, R.: Reformulation of the site-site interaction theory for molecular fluids, **71**, 945
BOUGHEY, J.D., *see* Goodwin, S.P.
BOULU, L.G., and KOZAK, J.J.: Simulations of energy transfer and trapping in two-dimensional disordered systems, **62**, 1449
BOULU, L.G., and KOZAK, J.J.: Simulations of fluorescence quenching using theoretical models of energy and electron transfer in random arrays. Applications to experiments on monolayers of chlorophyls and quinones, **65**, 193
BOUTEILLER, Y., MIJOULE, C., NIZAM, M., BARTHELAT, J.C., DAUDEY, J.P., PELISSIER, M., and SILVI, B.: Extended gaussian-type valence basis sets for calculations involving non-empirical core pseudopotentials, **65**, 295
BOUTIN, A., *see* Rousseau, B.
BOVENSMANN, H., KNOCKEL, H., and TIEMANN, E.: Hyperfine structure investigations of the excited AO^+ state of TlI, **73**, 813
BOWDEN, G.J., MARTIN, J.P.D., and PRANDOLINI, M.J.: Non-square tensor algebra and application in the NMR of multiply connected spin systems: I, **74**, 985
BOWDEN, G.J., MARTIN, J.P.D., and SEPAROVIC, F.: Tensorial sets for coupled pairs of spin-½ nuclei, **70**, 581
BOWDEN, G.J., and PRANDOLINI, M.J.: Non-square tensor algebra applications in the NMR of multiply connected spin systems: II, **74**, 999
BOWDEN, Z.A., *see* Andreani, C.
BRAGA, J.P., GUO, H., MURRELL, J.N., and DUNNE, L.J.: A comparative study of quantum mechanical and classical trajectory calculations for an $A + BC$ collinear non-adiabatic collisions, **65**, 909
BRAMLEY, M.J., GREEN, W.H. JR., and HANDY, N.C.: Vibration-rotation coordinates and kinetics energy operators for polyatomic molecules, **73**, 183
BRAMLEY, M.J., *see* Pinnavaia, N.
BRAMLEY, M.J., *see* Su, M-D.
BRAŃKA, A.C., and WOJCIECHOWSKI, K.W.: Monte Carlo simulation of hard cyclic pentamers in two dimensions. Equation of state and structural properties, **72**, 941
BRAŃKA, A.C., and WOJCIECHOWSKI, K.W.: Monte Carlo simulations of hard cyclic pentamers in two dimensions. Translational-rotational coupling in the orientationally disordered phase, **78**, 1513
BRAS, W., *see* van der Marel, C.
BRÄUCHLE, c., *see* Trentini, F.V.

BRAULT, J.W., *see* Rogers, S.A.
BRAUN, D., GALLHUBER, E., HENSLER, G., and YERSIN, H.: Site selective spectra of the lowest excited states of $[Os(bpy)_3]^{2+}$ in $[Ru_{1-x}Os_x(bpy)_3]X_2(X = PF_6, AsF_6, SbF_6)$, **67**, 417
BRAZIER, C.R., *see* Rogers, S.A.
BRENAN, G.P., and EVANS, R.: Free energy functionals and the uniform hard-sphere fluid, **73**, 789
BRESGUNOV, A. YU., DUBINSKY, A.A., POLUEKTOV, O.G., LEBEDEV, YA. S., and PROKOF'EV, A.I.: The structure of phenoxyl radicals as studied by 2 mm band ESR, **75**, 1123
BRESME, F., *see* Abascal, J.L.F.
BREUILLARD, C., *see* Dreyfus, C.
BREY, J.J., *see* Castaño, F.
BRIDGEMAN, A.J., and GERLOCH, M.: A cellular ligand-field model for *l-l* spectral intensities. VI. Planar tetrahaloplatinum(II) and tetrahalopalladium(II) ions, **79**, 1195
BRIGGS, D., *see* Beamson, G.
BRIGGS, J.M., *see* Jorgensen, W.L.
BRILLIANTOV, N.V., and VOSTRIKOVA, N.G.: Rotational motion of Brownian particles with surface charge, **77**, 957
BRINCK, T., MURRAY, J.S., and POLITZER, P.: Quantitative determination of the total polarity (charge separation) in molecules, **76**, 609
BROCKS, G.: The calculation of resonance by an L^2 method; rotational resonances of H_2Ar, **62**, 1483
BROCKS, G., and VAN KOEVEN, D.: The calculation of van der Waals vibrational and rotational states of atom-large molecule complexes, with Ar-fluorene as an example, **63**, 999
BRODE, S., and MCDONALD, I.R.: Excess thermodynamic properties of liquid mixtures of methane and perfluoromethane, **65**, 1007
BRÓDKA, A., *see* Nikiel, L.
BRÓDKA, A., *see* Stryczek, B.
BRÓDKA, A., STRYCZEK, B., NIKIEL, L., and WRZALIK, R.: The microscopic friction tensor of reorientational motion in liquid benzene, **65**, 619
BRÓDKA, A., and WRZALIK, R.: Fermi resonance in liquid methyl bromide, **73**, 1101
BRODKA, A., and ZERDA, T.W.: A molecular dynamics simulation of sulphur hexafluoride, **76**, 103
BRODSKAYA, E.N., and RUSANOV, A.I.: The molecular dynamics simulation of water clusters, **62**, 251
BRODSKAYA, E.N., and RUSANOV, A.I.: Molecular-dynamics simulation of water clusters with ions, **71**, 457
BROMMER, M., ROSMUS, P., CARTER, S., and HANDY, N.C.: Rovibronic $^2B_1(\Pi_u)$-$^2A_1$ spectrum of the BH_2 radical, **77**, 549
BRONDEAU, J., *see* Elbayed, K.
BROOKS, B.R., *see* Pastor, R.W.
BROOMFIELD, K., and LAMBERT, R.M.: Model studies of oxygen chemisorption on silver surfaces using an AgO_2 cluster, **66** 421
BROQUIER, M., *see* Aroui, H.
BROQUIER, M., LEFEVRE, G., PITTMAN, M., PICARD-BERSELLINI, A., CHEVALIER, M., and BILLING, G.: Transfer of rotational population in NH_3 by infrared-infrared double resonance, **79**, 1103
BROUARD, M., MARTINEZ, M.T., O'MAHONY, J., and SIMONS, J.P.: Energy and angular momentum disposals in the vibrationally mediated photodissociation of HOOH and HOOD. Intramolecular properties via photofragment mapping, **69**, 65
BROUARD, M., MARTINEZ, M.T., and O'MAHONY, J.: Fragment pair correlations in the vibrationally mediated photodissociation of H_2O_2: rotation-vibration coupling in the third OH stretching overtone state, **71**, 1021
BROWN, A., *see* Baggott, J.E.
BROWN, C.A., GERLOCH, M., and MCMEEKING, R.F.: A cellular ligand-field model for '*l-l*' spectra intensities. I. Formalism and parameters, **64**, 771
BROWN, C.A., DUER, M.J., GERLOCH, M., and MCMEEKING, R.F.: A cellular ligand-field model for '*l-l*' spectral intensities. II. Applications within the *d* block, **64**, 793
BROWN, C.A., DUER, M.J., GERLOCH, M., and MCMEEKING, R.F.: A cellular ligand-field model for '*l-l*' spectral intensities. III. Correlations of parameters with structure and bonding, **64**, 825
BROWN, J., *see* Burghardt, I.
BROWN, J.M., *see* Carrington,
BROWN, J.M., *see* Lipus, K.
BROWN, J.M., *see* Petri, M.
BROWN, J.M., *see* Seebass, W.

BROWN, J.M., *see* Steimle, T.C.
BROWN, J.M., *see* Towle, J.P.
BROWN, J.M., *see* Woodward, D.R.
BROWN, M.F.: Anisotropic nuclear spin relaxation of cholesterol in phospholipid bilayers, **71**, 903
BROWN, M.F., SALMOND, A., HENRIKSSON, U., and SODERMAN, O.: Frequency dependent ^{2}H N.M.R. relaxation rates of small unilamellar phospholipid vesicles, **69**, 379
BROWN, M.S., and FROMMHOLD, L.: Polarized light scattering from pairs of anisotropic linear molecules (H_2-H_2, D_2-D_2), **66**, 527
BROWN, M.S., FROMMHOLD, L., and BIRNBAUM, G.: About an information theoretical spectra line shape proposed for the collision induced spectroscopies, **62**, 907
BROWN, M.S., FROMMHOLD, L., and BIRNBUAM, G.: Reply to comment on 'About an information theoretical line shape proposed for the collision induced spectroscopies', **64**, 1001
BROWN, R.D.,DYALL, K.G., GODFREY P.D., and MCNAUGHTON, D.: Spin-rotation hyperfine structure in the rotation spectrum of ^{77}Se-selenoformadehyde, **61**, 783
BROWN, R.D., and HEAD-GORDON, M.P.: *Ab initio* calculation of ^{14}N nuclear quadrupole coupling constants, **61**, 1183
BROWN, R.D., GODFREY, P.D., MCNAUGHTON, D. and YAMANOUCHI, K.: Hyperfine structure in thioformaldehyde, **62**, 1429
BROYER, M., *see* Perrott, J.P.
BROYER, M., CABAULD, B., HOAREEAU, A., MELINON, P., RAYANE, D., and TRIBOLLETT, B.: Velocity slip measurements of bismuth clusters produced by the inert gas condensation techniques, **62**, 559
BRUIN, C., *see* Nijmeijer, M.J.P.
BRUNA, P.J., *see* Anglada, J.
BRUNA, P.J., *see* Baoqi Meng
BRUNA, P.J., and GREIN, F.: Low-lying electronic states of Ge_2^+ : a pseudopotential MRD-CI study, **74**, 1133
BRUNA, P.J., and GREIN, F.: MRD-CI study on the isomers and HSiO. I. Relative stability and electronic spectra, **63**, 329
BRUNA, P.J., and HIRSCH, G.: Characterization of the excited electronic states of the SH radical by *ab initio* methods, **61**, 1359
BRUNET, J.-P., *see* Chapuisat, X.
BRUNETTI, B., *see* Aguilar, A.
BRUNNER, H., *see* Kümmerlen, J.
BRUSTOLON, M., *see* Caciuffo, R.
BRUSTOLON, M., CASSOL, T., MICHELETTI, L. and SEGRE, U.: ENDOR studies of methyl dynamics in molecular crystals, **61**, 249
BRUSTOLON, M., MANIERO, A.L., and SEGRE, U.: An ENDOR study of the slow intramolecular motions in the CH_2COO^- radical, **65**, 447
BRUSTOLON, M., *see* Maniero, A.L.
BUCKINGHAM, A.D., *see* Fowler, P.W.
BUCKINGHAM, A.D., *see* McDowell, S.A.
BUCKNALL, R.E., CLARKE, S.M., SHAPTON, R.A., and THOMAS, R.K.: The structure of a methyl iodide monolayer adsorbed on graphite, **67** 439
BUCHNER, M., and LADANYI, B.M.: Molecular dynamics algorithm for flexible molecules using normal coordinates, **73**, 1127
BUCHNER, R., and YARWOOD, J.: Far-infrared studies of molecular dynamics and interactions in N,N-dimethylformamide, **71**, 65
BUENKER, R.J.: Evidence from the special relativity and blackbody radiation theories for the existence of photons possessing zero kinetic energy, **76**, 277
BUENKER, R.J.: Exponentially damped Breit-Pauli Hamiltonian for the description of positronium decay and other higher energy processes, **77**, 1095
BUENKER, R.J., *see* Alvarez-Collado, J.R.
BUENKER, R.J., *see* Bhanuprakash, K.
BUENKER, R.J., *see* Hirsch, G.
BUENKER, R.J., *see* Jensen, P.
BUENKER, R.J., *see* Li, Y.
BUENKER, R.J., *see* Perić, M.
BUENKER, R.J., *see* Petrongolo, C.
BUENKER, R.J., *see* Theodorakopoulos, G.

BUJÁN-NÚÑEZ, M.C., *see* López-Quintela, M.A.
BUJÁN-NUÑEZ, M.C., and DICKINSON, E.: Brownian dynamics model of deformable particle absorption, **80**, 431
BUOTEMPO, U., *see* Bellissent-Funel, M.-C.
BUOTEMPO, U., FILABOZZI, A., and MASELLI, P.: Collision induced fundamental band of N_2 and N_2-Ar mixtures, **67**, 517
BURDEN, F.R., and CUNO, A.: A variational description of the rotational and vibrational states of triatomic molecules using numerical wavefunctions, **62**, 33
BURDEN, F.R., and SUTCLIFFE, B.T.: Three-body calculations in laboratory-fixed hyperspherical coordinates: convergence properties using numerical wavefunctions as applied to the positronium ion d_e, **80**, 383
BURENIN, A.V.: Optimum rational versions of effective rotational Hamiltonian operator of the symmetric top-type molecule. Application to the PH_3 molecule in the ground state, **75**, 305
BÜRGER, H., see Lattanzi, F.
BÜRGER, H., *see* Najib, H.
BURGESS, A.N., *see* Hall, C.D.
BURGHARDT, I., KONRAT, R., and BODENHAUSEN, G.: Measurement of cross correlation of fluctuations of dipolar couplings and anisotropic chemical shifts by selective spin locking, **75**, 467
BURGHARDT, I., ZINK, L.R., FLETCHER, D.A., BROWN, J., and BEATTIE, I.R.: Nuclear hyperfine structure in the electronic spectrum of CuCl, **67**, 1401
BURIE, J., *see* Wlodarczak, G.
BURIE, J.-R., DAVIES, P.B., HANSFORD, G.M., MARTIN, N.A., GANG, J., and RUSSELL, D.K.: Diode laser infrared spectroscopy of jet-cooled hexacarbonyls of chromium, molybdenum, and tungsten, **74**, 919
BURNELL, E.E., *see* Delikatny, E.J.
BURNELL, E.E., *see* Li, K.Y.
BURNELL, E.E., *see* Ter Beek, L.D.
BURNELL, E.E., *see* Zimmerman, D.S.
BURTON, N.A., *see* Young, P.
BURYKIN, B.N., *see* Oshtrakh, M.I.
BUSAROW, K.L., *see* Dz-Hung Gwo
BUSCHER, H., *see* Marks, A.J.
BUSIGIN, A., and PHILLIPS, C.R.: Efficient Newton-Raphson and implicit Euler methods for solving the HNC equation, **76**, 89
BUSZKO, M.L., and ANDREW, E.R.: NMR study of solid lactic acid (2-hydroxypropanoic acid), **76**, 83
BYERS BROWN, W., and HORTON, T.V.: Hard-sphere perturbation theory for classical fluids to high densities, **63**, 125

CABAÇO, M.I., BESNARD, M., and YARWOOD, J.: Raman spectroscopic studies of vibrational relaxation and chemical exchange broadening in hydrogen bonded systems. 1. Investigation of relaxation processes in binary mixture of pyridine and ethanol, **75**, 139
CABAÇO, M.I., BESNARD, M., and YARWOOD, J.: Raman spectroscopic studies of vibrational relaxation and chemical exchange broadening in hydrogen bonded systems. 2. Analysis of the effect of exchange dynamics in the pyridine + ethanol system, **75**, 157
CABAUDC B., *see* Broyer, M.
CABEZAS, H., *see* Perry, R.L.
CABLE, J.W., *see* Figgis, B.N.
CACCAMO, C., and GIUNTA, G.: Microscopic theoretical description of phase stability in hard sphere Yukawa mixtures, **78**, 83
CACIUFFO, R., FRANCESCANGELI, O., GRECI, I., MELONE, S., GILLON, B., BRUSTOLON, M., MANIERO, A.L., AMORETTI, G., and SGARABOTTO, P.: Unpaired electron density in an indolinonic nitroxide radical as determined by polarized neutron diffraction, **74**, 905
CADOT, J.: Short-range radial contributions and symmetry properties of the intermolecular potential, **78**, 1143
CAĞIN, T., and PETTITT, B.M.: Molecular dynamics with a variable number of molecules, **72** , 169
CAILLOL, J.M., LEVESQUE, D., WEISS, J.J., KUSALIK, P.G., and PATEY, G.N.: A comparison between computer simulation and theoretical results for ionic solutions, **62**, 461

CAILLOL, J.M., LEVESQUE, D., WEISS, J.J., PERKYNS, J.S., and PATEY, G.N.: A theoretical study of a polar-polarizable model for liquid ammonia, **62**, 1225

CAILLOL, J.M., LEVESQUE, D., and WEISS, J.J.: Monte Carlo simulation of an ion-dipole mixture. A convergence study, **69**, 199

CALEF, D.F., *see* Madura, J.D.

CALEF, D.F., *see* Nichols III, A.L.

CALLEJA, M., NORTH, A.N., POWLES, J.G. and RICKAYZEN, G.: The structure of fluids confined to spherical pores: theory and simulation, **73**, 973

CALLEJA, M., and RICKAYZEN, G.: The structure of a confined fluid of cylindrical 'molecules': simulation and theory, **76**, 693

CALLEJA, M., and RICKAYZEN, G.: Modified Meister-Kroll density functional applied to the structure of an inhomogeneous hard sphere fluid, **79**, 809

CALLOMON, J.H., *see* Aarts, J.F.M.

CALMETTES, P., *see* Cartailler T.

CALOGERACOS, A., and CASTILLEJO, L.: A derivation of molecular vibrational-rotational Hamiltonians, **80**, 1359

CALVO, C., *see* Desouter-Lecomte, M.

CALVO HERNÁNDEZ, A., *see* Velasco, S.

CALVO HERNÁNDEZ, A., VELASCO, S., PÉREZ, J., GÜÉMEZ, J., and WHITE, J.A.: Non-markovian far-infrared spectra of HF in liquid SF_6, **65**, 1001

CAMINITI, R., CILLOCO, F., and FELICI, R.: X-ray and neutron diffraction studies of the hydration of SeO_4^{2-} and CrO_4^{2-} anions by isomorphic substitution, **76**, 681

CAMINATI, W., DAMIANI, D., CORBELLI, G., VELINO, B., and BOCK, C.W.: Microwave spectrum and *ab initio* calculations of ethylbenzene: potential energy surface of the ethyl group torsion, **74**, 885

CAMINATI, W., DAMIANI, D., CORBELLI, G., and FAVERO, L.B.: Ring puckering motion in indan: a microwave spectroscopy study, **75**, 857

CAMINATI, W., DAMIANI, D., and FAVERO, L.B.: Non-planarity and barrier to ring puckering in phthalan, **79**, 699

CAMINATI, W., FANTONI, A.C., MANESCALCHI, F., and SCAPPINI, F.: Methyl and skeletal torsion interaction in normal propyl fluoride, **64**, 1089

CAMINATI, W., FAVERO,, L.B., VELINO, B., and ZERBETTO, F.: A study of the large amplitude motions of indoline through microwave spectroscopy and *ab initio* calculations. Evidence of ring puckering and butterfly motion coupling, **78**, 1561

CAMINATI, W., MELANDRI, S., CORBELLI, G., FAVERO, L.B., and MEYER, R.: Chair conformation and barrier to ring puckering in 1,3-benzodioxole, **80**, 1297

CAMINATI, W., VELINO, B., and FANTONI, A.C.: High resolution microwave spectrum and torsional potential energy surfaces of *trans*-crotyl alcohol, **61**, 1269

CAMY-PEYRET, C., *see* Lechuga-Fossat, L.

CAMY-PEYRET, C., *see* Perrin, A.

CAMY-PEYRET, C., FLAUD, J.-M., N'GOM, A., and JOHNS, J.W.C.: The three fundamental bands υ_2, υ_1 and υ_3 of $D_2{}^{32}S$ and the υ_2 band of $D_2{}^{34}S$, **65**, 649

CAMY-PEYRET, C., FLAUD, J.-M., N'GOM, A., and JOHNS, J.W.C.: The υ_2 band of $HD^{32}S$, **67**, 693

CANALES, M., *see* Padró, J.A.

CANESSA, E. D'AGUANNO, B., WEYERICH, B., and KLEIN, R.: Towards an understanding of the static structure of suspensions of ionic rod-like macromolecules, **73**, 175

CANESSA, E., GONZALEZ, D.J., GRIMSON, M.J., and SILBERT, M.: Variational theory for the phase diagram of sterically stabilized colloidal dispersions, **64**, 207

CANESSA, E., GRIMSON, M.J., and SILBERT, M.: Volume dependent forces in charge stabilized colloidal crystals, **64**, 1195

CANESSA, E., GRIMSON, M.J., and SILBERT, M.: Theory of phase equilibria in polymer stabilized colloidal suspensions, **67**, 1153

CANET, D., *see* Elbayed, K.

CANET, D., *see* Jalabert, D.

CANET, D., *see* Tekely, P.

CANIPAROLI, J.P., GRASSI, A., and CHACHATY, C.: Correlated internal motions and nuclear spin relaxation in lamellar mesophase, **63**, 419

CARIGNAN, Y.P., *see* Vladimiroff, T.

CARLEER, M., *see* Ndikumana, T.

CARLI, B., *see* Perrin, A.

CARLILE, C.J., *see* Fillaux, F.
CARLILE, C.J., JAMIE, I.M., LOCKHART, G., and WHITE, J.W.: Two-dimensional caesium-ammonia solid solutions in $C_{28}Cs(NH_3)_x$, **76**, 173
CARLONI, P., *see* Maniero, A.L.
CARLSTRÖM, G., and HALLE, B.: Nuclear spin quenching. A new probe of exchange kinetics and droplet size in disperse systems, **64**, 659
CAROLOTTI, M., *see* Perrin, A.
CARPENTIER, L., BÉE, M., GIROUD-GODQUIN, A.M., MALDIVI, P., and MARCHON, J.C.: Alkyl chain motions in columnar mesophases. A quasielastic neutron scattering study of dicopper tetrapalmitate, **68**, 1367
CARPENTIER, L., *see* Decressain, R.
CARPIENTIER, L., *see* Giroud-Godquin, A.M.
CARRINGTON, A., MCNAB, I.R., and MONTGOMERIE, C.A.: Vibration-rotation spectroscopy of the HD^+ ion near the dissociation limit. IV. Nuclear hyperfine structure in the v = 18-16 band, **64**, 679
CARRINGTON, A., MCNAB, I.R., and MONTGOMERIE, C.A.: Vibration-rotation spectroscopy of the HD^+ ion near the dissociation limit. V. Direct measurement of the asymmetric electron distribution in v = 21, **64** , 983
CARRINGTON, A., MCNAB, I.R., and MONTGOMERIE, C.A.: Spectroscopic observation of HD^+ in the v = 22 level, **65**, 751
CARRINGTON, A., MCNAB, I.R., and MONTGOMERIE, C.A.: Radiofrequency/infrared double resonance spectroscopy of the HD^+ ion, **66**, 519
CARRINGTON, A., MCNAB, I.R., MONTGOMERIE, C.A., and BROWN, J.M.: Microwave spectra of the HD^+ and D_2^+ ions at their dissociation limits, **66**, 1279
CARRINGTON, A., MCNAB, I.R., MONTGOMERIE, C.A., and KENNEDY, R.A.: Electronic spectrum ($2p\sigma_u$-$1s\sigma_g$) of the D_2^+ion, **67**, 711
CARRINGTON, A., MCNAB, I.R., MONTGOMERIE-LEACH, C.A., and KENNEDY, R.A.: Vibration-rotation spectroscopy of the HD^+ ion near the dissociation limit. Part VI. Nuclear hyperfine interactions, **72**, 735
CARRINGTON, JR, T.: Perturbation theory for bending potentials, **70**, 757
CARRINGTON , JR, T., *see* Charron, G.
CARRINGTON, JR, T., *see* McNichols, A.
CARROLL, M.T., and BADER, R.F.W.: An analysis of the hydrogen bond in BASE-HF complexes using the theory of atoms in molecules, **65**, 695
CARROLL, M.T., CHANG, C., and BADER, R.F.W.: Prediction of the structures of hydrogen-bonded complexes using the laplacian of the charge density, **63**, 387
CARTAILLER, T., CALMETTES, P., KUNZ, W., TURQ, P., and ROSSY-DELLUC, S.: Cryptates as model Brownons. I. Small-angle neutron scattering experiments, **80**, 833
CARTER, S., *see* Brommer, M.
CARTER, S., HANDY, N.C., ROSMUS, P., and CHAMBAUD, G.: A variational method for the calculation of spin-rovibronic levels of Renner-Teller triatomic molecules, **71**, 605
CARTER, S., SENEKOWITSCH, J., HANDY, N.C., and ROSMUS, P.: Calculations of the rovibrational absorption transition probabilities in triatomic molecules, **65**, 143
CARTER, S., *see* Li, Y.
CASSOL, T., *see* Brustolon, M.
CASTAÑO, F., BREY, J.J., and SANTOS, A.: Nonclassical critical exponents in the mean spherical approximation, **66**, 695
CASTEX, M.C., *see* Maïnos, C.
CASTILLEJO, L., *see* Calogeracos, A.
CASTILLO, R., VILLAVERDE, A., and OROZCO, J.: Prediction of transport properties for Lennard-Jones fluids and their binary mixtures using the effective-diameter hard-sphere kinetic theory, **74**, 1315
CASTILLO, R., and OROZCO, J.: Prediction of transport properties of dense molecular fluids using the effective diameter hard sphere theory. Perturbation method, **79**, 343
CATALIOTTI, R.S., *see* Giorgina, M.G.
CATALIOTTI, R.S., *see* Sassi, P.
CATLOW, C.R.A., *see* Pavlides, P.
CAUSÀ, M., *see* Salasco, L.
CAUSÀ, M., *see* Silvi, B.
CAVAGNAT, D., *see* Lassegues, J.C.

CELEBRE, G., DE LUCA, G., LONGERI, M., and EMSLEY, J.W.: The barrier to internal rotation in benzyl fluoride investigated using the N.M.R. spectra of samples dissolved in liquid crystalline solvents, **67**, 239

CELEBRE, G., LONGERI, M., and EMSLEY, J.W.: The nature of the internal rotational barrier in benzyl chloride. An interpretation of the dipolar coupling constants obtained from the analysis of the proton N.M.R. spectra of samples dissolved in liquid crystal solvents, **64**, 715

CELEBRE, G., LONGERI, M., RUSSO, N., AVENT, A.G., EMSLEY, J.W., and SINGLETON, V.N.: The potential function for rotation about the phenyl-C bond in 3,5-dibromoethylbenzene. An investigation by proton N.M.R. of a sample dissolved in a nematic solvent, **65**, 391

CELII, F.G., RÖSSLEIN, M., HANRATTY, M.A., and MAIER, J.P.: Rotational analysis of the $B^2\Pi_{3/2} \leftarrow X^2\Pi_{3/2}$ laser excitation spectrum of chlorocyanide cation, **62**, 1435

CELII, F.G., see Hanratty, M.A.

CÉOLIN, R., *see* André, D.

CEULMANS, R., and VOS, I.: The vibrations of annular and globular molecules: theory, **72** , 1051

CHACHAM, H., and MOHALLEM, J.R.: Fast Hartree-Fock calculations by simulated dynamics. Part I: Formulation and a test application, **70**, 391

CHACHATY, C., *see* Caniparoli, J.P.

CHAHID, A., GARCIA-HERNANDEZ, M., PRIETO, C., BERMEJO, F.J., ENCISO, E., and MARTÍNEZ, J.L.: Inelastic neutron and light scattering studies on liquid sulphur dioxide, **78**, 821

CHAKRABORTI, P.K., *see* Talukdar, R.

CHAKRAVARTY, C., and CLARY, D.C.: Ion-dipole fragmentations, **67**, 1099

CHALAM, M.K., *see* de Miguel, E.

CHAŁASIŃSKI, G., *see* Gutowski, M.

CHAŁASIŃSKI, G., and SZCZĘŚNIAK, M.M.: On the connection between the supermolecular Møller-Plesset treatment of the interaction energy and the perturbation theory of intermolecular forces, **63**, 205

CHAMBAUD, M.K., *see* Carter, S.

CHAMBERS, A.V., and CHILD, M.S.: Barrier effects on the vibrational predissociation of HD_{2+}, **65**, 1337

CHAMBRON, J., *see* Grucker, D.

CHAMPENEY, D.,C., *see* Garawi, M.

CHAMPION, J.P., *see* Tyuterev, V.G.

CHAN, K.-Y., GUBBINS, K.E., HENDERSON, D., and BLUM, L.: Monte Carlo and simple theoretical calculations for ion-dipole mixtures, **66**, 299

CHAN, KWONG-YU *see* Lo, Wai Yin

CHANDLER, D., *see* Kurtović, Z.

CHANDLER, G.S., *see* Barnes, L.A.

CHANDRASEKHARAN, V., *see* Le Duff, Y.

CHANG, C., *see* Carroll, M.T.

CHANTELOUP, J.-C., *see* Berg, L.-E.

CHAO, K.C., *see* Lee, R.J.

CHAPELA, G.A., *see* Alejandre, J.

CHAPMAN, W.G., *see* Etesse, P.

CHAPMAN, W.G., *see* Ghonasgi, D.

CHAPUISAT, X., BELAFHAL, A., NAUTS, A., and IUNG, C.: A comment on recent proposals for the calculation of vibration-rotation energies in more-than-three atom molecules, **77**, 947

CHAPUISAT, X., NAUTS, A., and BRUNET, J.-P.: Exact quantum molecular Hamiltonians. Part I. Application to the dynamics of three particles, **72**, 1

CHAPUISAT, X.: Exact quantum molecular Hamiltonians. II. On the choice of the moving frame of reference. The principal axis system, **72**, 1233

CHAPUISAT, X., *see* Schneider, F.

CHAPMAN, S., *see* Corey, G.C.

CHAPMAN, W.G., *see* Joslin, C.G.

CHAPMAN, W.G., *see* Jackson, G.

CHAPMAN, W.G., JACKSON, G., and GUBBINS K.E.: Phase equilibria of associating fluids. Chain molecules with multiple bonding sites, **65**, 1057

CHARRON, G., and CARRINGTON JR, T.: A Fourier-Lanczos method for calculating energy levels without storing or calculating matrices, **79**, 13

CHATTERJEE, A., and WIDOM, B.: Model lamellar-lamellar phase equilibria, **80**, 741

CHAVE, A., *see* Barreau, A.

CHAZIN, W.J., *see* Palmer, A.G. III.

CHECHETKIN, V.R., and LUTOVINOV, V.S.: On the Hall number in dilute electrolyte solutions, **68**, 979
CHEN, A., and HIRTZEL, C.S.: Monte Carlo simulations of reactive and non-reactive desorption of molecules from solid surfaces, **79**, 757
CHEN, A.F.T., *see* Wang, S.P.
CHEN, W.-H., RIECKHOFF, K.E., and VOIGT, E.-M.: Zeeman effect of the platinum phthalocyanine n-π^* phosphorescences, **62**, 541
CHEN, W.-H., RIECKHOFF, K.E., VOIGT, E.-M., and THEWALT, M.L.W.: Double fluorescence lifetimes of metal-free phthalocyanine in a mixed-solvent Shpol'skii matrix at 4.2K, **67**, 1439
CHEN, W.-H., HUANG, T.-H., RIECKHOFF, K.E., and VOIGT, E.M.: Electronic spectra and Zeeman effect of ruthenium phthalocyanine in Shpol'skii matrices, **68**, 341
CHEN, X.S., and FORSTMANN, F.: The phase instability of molecular fluid mixtures: dipolar and neutral hard spheres, **76**, 1203
CHEN, X.S., *see* Kasch, M.
CHEVALEYRE, J., *see* Perrot, J.P.
CHEVALIER, M., *see* Broquier, M.
CHEVALIER, R., *see* Aroui, H.
CHEWTER, L.A., SMITH, I.W.M., and YARWOOD, G.A.: A high resolution FTIR spectroscopic study of the ν_1 (n = 1-4) bands of N_2O_3, **63**, 843
CHIALVO, A.A.: Excess properties of liquid mixtures from computer simulation: a coupling parameter approach to the determination of their dependence on molecular asymmetry, **73**, 127
CHIALVO, A.A., and CUMMINGS, P.T.: Unified expression for the calculation of thermal conductivity in the canonical ensemble, **78**, 791
CHIBOTARU, L.F., *see* Bersuker, G.I.
CHICCOLI, C., *see* Biscarini, F.
CHICCOLI, C., PASINI, P., BISCARINI, F., and ZANNONI, C.: The P_4 model and its orientational phase transition, **65**, 1505
CHIDICHIMO, G., IMBARDELLI, D., LONGERI, M., and SAUPE, A.: Conformation of ethylene glycol dissolved in a nematic-lyotropic solution: an N.M.R. analysis, **65**, 1143
CHIDICHIMO, G., FORMOSO, P., GOLEMME, A., and IMBARDELLI, D.: Conformation of succinic acid; its pH dependence by Licry-NMR analysis, **79**, 25
CHIDICHIMO, G., *see* Imbardelli, D.
CHIERICO, A., *see* Mognaschi, E.R.
CHIEUX, P., *see* Alvarez, M.
CHIEUX, P., *see* Bausenwein, T.
CHIEUX, P., *see* Jung, W.G.
CHIEUX, P., *see* Mittag, U.
CHIEUX, P., *see* Neuefeind, J.
CHIEW, Y.C.: Percus-Yevick integral-equation theory for athermal hard-sphere chains. Part I: Equations of state, **70**, 129
CHIEW, Y.C.: Percus-Yevick integral equation theory for athermal hard-sphere chains. II. Average intermolecular correlation functions, **73**, 359
CHIHARA, H., *see* Inaba, A.
CHILD, M.S.: Analysis of a complex absorbing barrier, **72**, 89
CHILD, M.S., *see* Chambers, A.V.
CHILD, M.S., *see* Gilbert, R.D.
CHILD, M.S., *see* Hirst, D.M.
CHILD, M.S., *see* Lefebvre, R.
CHINGAS, G.C., *see* Suter, D.
CHMELKA, B.F., *see* McCormick, A.V.
CHO, H., MUELLER, K.T., SHAKA, A.J., and PINES, A.: Frequency selective N.M.R. pulse sequences generated by iterative schemes with multiple fixed points, **67**, 505
CHOKAPPA, D.K., and CLANCY, P.: A computer simulation study of the melting and freezing properties of a system of Lennard-Jones particles. I. Melting the solid, **61**, 597
CHOKAPPA, D.K., and CLANCY, P.: A computer simulation study of the melting and freezing properties of a system of Lennard-Jones particles. II. Cooling the liquid, **61**, 617
CHOKAPPA, D.K. and CLANCY, P.: The influence of an interface in the promotion of melting, **65**, 97
CHOU, S.Y., *see* Yu, J.-T.
CHRISTIANSEN, P.A., *see* Walker, E.C.

CHRISTMANN, K.: Invited Article. The interaction of hydrogen with metal surfaces of two-fold symmetry, **66**, 1
CHRISTOV, S.G.: Quantum decay rates in dense media, **76**, 1241
CHUANG, T.J., *see* Yamada, T.
CHUAQUI, C.E., *see* Slee, T.
CHUDINOV, G.E., *see* Basilevsky, M.V.
CHUNG, CHUN-WA, and WIMPERIS, S.: Measurement of spin-5/2 relaxation in biological and macromolecular systems using multiple-quantum NMR techniques, **76**, 47
CHUPKA, W.A., *see* Gauyacq, D.
CIBSTA, S., *see* Petsalakis, I.D.
CICCOTTI, G., *see* Depaepe, J.-M.
CICCOTTI, G., *see* Melchionna, S.
CICCOTTI, G., *see* Paolini, G.V.
CICHOCKI, B., and FELDERHOF, B.U.: Electrostatic interactions in thin film Coulomb systems with periodic boundary conditions, **67**, 1373
CILLOCO, F., *see* Caminiti, R.
CILLOCO, F., *see* Felici, R.
CINA, J.A., and SCHOFIELD, S.A.: Molecular excitations and the quantum adiabatic phase for a nuclear spin, **67**, 271
CLAIRET, F., *see* Goulay, A.M.
CLANCY, P., *see* Chokappa, D.K.
CLANCY, P., *see* Holcomb, C.D.
CLARKE, S.M., *see* Bucknall, R.E.
CLARKE, S.M., *see* Inaba, A.
CLARKE, S.M., *see* Morishige, K.
CLARKE, S.M., and THOMAS, R.K.: The structure of a bromomethane monolayer adsorbed on graphite, **72**, 413
CLARY, D.C., *see* Agg, P.J.
CLARY, D.C., *see* Chakravarty, C.
CLEAVER, D.J., and ALLEN, M.P.: Computer simulation of liquid crystal films, **80**, 253
CLEPHAS, M.P.J.W., *see* Willems, J.-P.
CLERHAUX, C., and COLIN, R.: The 3d Rydberg state of the BeH molecule, **72**, 471
CLIFFE, A.J., *see* Randall, R.W.
CLIFFORD, P., *see* Atkinson, R.A.
CLIFFORD, P., *see* Green, N.J.B.
CLOUGH, S.: The topology of methyl rotation and gauge theory in solids, **68**, 1255
CLOUGH, S., HORSEWILL, A.J., JOHNSON, M.R., and TOMSAH, I.B.I.: Resonant broadening of NMR line shapes of tunnelling methyl groups at level anticrossings, **78**, 781
COCKCROFT, J.K., *see* Jouanneaux, A.
CODDENS, G., *see* Guillaume, F.
COFFEY, W.T., *see* Corcoran, P.M.
COFFEY, W.T., CORCORAN, P.M., and EVANS, M.W.: On the existence of far-infrared absorption peaks in the complex polarizability of the itinerant oscillator model of polar fluids, **61**, 15
COHEN, R.C., *see* Dz-Hung Gwo
COHEN, R.C., *see* Pringle, W.C.
COHEN DE LARA, E.R.: Experimental and theoretical determination of vibrational frequency shifts of diatomic molecules adsorbed in NaA zeolite. Interaction potential and its derivatives with respect to the internal coordinate of H_2, D_2, N_2, O_2, **66**, 479
COHEN DE LARA, E., GOULAY, A.M., SOUSSEN-JACOB, J., and KAHN, R.: Effect of an electric field on a methane molecule. II. Infrared intensity of the components of the splitting of the υ_3 vibrational mode, **76**, 1049
COHEN DE LARA, E., *see* Goulay, A.M.
COHEN DE LARA, E., *see* Soussen-Jacob, J.
COLE, W.A., and WAKEHAM, W.A.: Application of thermodynamic perturbation theory to a hexadecapolar fluid, **67**, 1167
COLETTA, F., MORO, G., and NORDIO, P.L.: Mobility of alklyl chains in quaternary ammonium salts, **61**, 1259
COLIN, R., *see* Clerbaux, C.
COLIN R., *see* Ndikumana, T.

COLLIGIANI, A., PINZINO, C., and ANGELON, R.: ENDOR study of a solitonic phase in a γ-irradiated single crystal of the malonic acid-urea 1:1 adduct, **62**, 97

COLPA, J.P., *see* Temme, F.P.

COLSON, S.D., *see* Gauyacq, D.

COLT, J.R., and SCUSERIA, G.E.: A coupled cluster study of the equilibrium bond distance in methane, **75**, 1199

COMBEN, E.R., *see* Seebass, W.

COOK, D.B., FOWLER, P.W., and PICKUP, B.T.: Variational freedom in self-consistent field calculations with basis sets, **80**, 213

COONEY, W.R., THOMPSON, S.M., and GUBBINS, K.E.: Virial coefficients for the hard oblate spherocylinder fluid, **66**, 1269

COOPER, D.L., *see* Barnard, S.A.

COOPER, D.L., *see* Raos, G.

COOPER, D.L., *see* Sironi, M.

COOPER, G., GREEN, J.C., and PAYNE, M.P.: Relative partial photoionization cross-sections and photoelectron branching ratios of the valence-bands of the group VIII metallocenes of iron, ruthenium and osmium, **63**, 1031

COPLAN, M.A., *see* McMillan, K.

CORBELLI, G., *see* Caminati, W.

CORCORAN, P.M., *see* Coffey, W.T.

CORCORAN, P.M., COFFEY, W.T., and EVANS, M.W.: On the calculation of the electric polarizability for the itinerant oscillator model. A comparison of numerical FFT techniques with approximate analytical formulae, **61**, 1

CORCORAN, P.M., and VIJ, J.K.: On the temperature dependence of the equal frictions itinerant oscillator model. Comparison with experimental observations on methyl chloride, **63**, 477

CORDERO, N.A., ALONSO, J.A. LOPEZ, J.M., and MARCH, N.H.: Dissociation energy of alkali metal clusters related to inhomogeneous electron gas theory, **79**, 393

COREY, G.C., MCCOURT, F.R.W., and CHAPMAN, S.: A comparison between calculated and experimental relaxation phenomena in binary gaseous mixtures. N_2-He, Ne and Ar, **62**, 875

COREY, G.C., MCCOURT, F.R.W., and MAITLAND, G.C.: A comparison between calculated and experimental transport coefficients of binary gaseous mixtures. N_2-He, Ne and Ar, **62**, 897

COREY, G.C., *see* Wong, C.C.K.

CORNELISSE, P.M.W., PETERS, C.J., and DE SWAAN AONS, J.: Simultaneous prediction of phase equilibria, interfacial tension and concentration profiles, **80**, 941

CORNELL, B., *see* Separovic, F.

CORONGIU, G., *see* Sciortino, F.

CORY, D.G., MILLER, J.B., TURNER, R., and GARROWAY, A.N.: Multiple-pulse methods of ^{1}H N.M.R. imaging of solids: second-averaging, **70**, 331

COSSART, D., *see* Cossart-Magos, C.

COSSART-MAGOS, C., JUNGEN, M., and LAUNAY, F.: High resolution absorption spectrum of CO_2 between 10 and 14 eV. Assignment of *nf* Rydberg series leading to a new value of the first ionization potential, **61**, 1077

COSSART-MAGOS, C., and COSSART, D.: Rotational band contours of the first electronic transition origin bands of p-xylyl and p-fluorobenzyl, **65**, 627

COSSART-MAGOS, C., LAUNAY, F., and PARKIN, J.E.: High resolution absorption spectrum of CO_2 between 1750 and 2000 Å. 1. Rotational analysis of nine perpendicular-type bands assigned to a new bent-linear electronic transition, **75**, 835

COSTA, C., *see* Magnasco, V.

COULING, V.W., and GRAHAM, C.: Higher-order dipole-dipole, dipole-quadrupole and field gradient contributions to the second light-scattering virial coefficient, **79**, 859

COUNSELL, C.J.R., EMSLEY, J.W., LUCKHURST, G.R., and SACHDEV, H.S.: Orientational order in the 4-n-alkyloxy-4′-cyanobiphenyls. A comparison between experiment and theory, **63**, 33

COURTEMANCHE, D.J., PASMORE, T.A., and VAN SWOL, F.: A molecular dynamics study of prefreezing. Hard spheres at a smooth hard wall, **80**, 861

COVENEY, F.M., STRANGE, J.H., and SMITH, E.G.: The measurement of electrophoretic mobility in surfactant systems using NMR, **75**, 127

COX, K.R., *see* Smit, B.

COXON, J.A., LI, M., and PRESUNKA, P.I.: Investigation of excited vibrational levels in the $X^2\Sigma^+$ state of CaOH and CaOD by resolved fluorescence spectroscopy, **76**, 1463

CRACKNELL, R.F., NICHOLSON, D., PARSONAGE, N.G., and EVANS, H.: Rotational insertion bias: a novel method for simulating dense phases of structured particles, with particular application to water, **71**, 931

CRACKNELL, R.F., NICHOLSON, D., and PARSONAGE, N.G.: Interbilayer repulsion in nonionic surfactant-water lamellar phases. 1. A Monte Carlo study of a dipole array model with discrete water molecules, **75**, 1023

CRACKNELL, R.F., NICHOLSON, D., and PARSONAGE, N.G.: Interbilayer repulsion in nonionic surfactant-water lamellar phases. 2. The role of binding site entropy, **75**, 1039

CRACKNELL, R.F., NICHOLSON, D., and QUIRKE, N.: A grand canonical Monte Carlo study of Lennard-Jones mixtures in slit shaped pores, **80**, 885

CRAVEN, C.J., HATTON, P.D., and PAWLEY, G.S.: Molecular dynamics study of reorientational motion in solid benzene, **79**, 1227

CRAVEN, C.J., *see* Rousseau, B.

CRAW, J.S., *see* De Almeida, W.B.

CREASEY, J.C., HATHERLY, P.A., JONES, H.M., LAMBERT, I.R., and TUCKETT, R.P.: Vacuum UV fluorescence excitation spectroscopy of BF_3 in the range 45-125 nm. Observation of new electronic transitions in the BF_2 free radical, **78**, 837

CREASEY, J.C., HATHERLEY, P.A., LAMBERT, I.R., and TUCKETT, R.P.: Vacuum UV fluorescence excitation spectroscopy of BCl_3 in the range 35-140 nm, **79**, 413

CREASEY, J.C., LAMBERT, I.R., TUCKETT, R.P., and HOPKIRK, A.: Vacuum UV spectroscopy and dynamics of CHF_3: analysis of emissions and evidence for parent ion emission, **71**, 1355

CREASEY J.C., LAMBERT, I.R., TUCKETT, R.P., and HOPKIRK, A.: Vacuum UV spectroscopy and dynamics of CF_3Cl, CF_2Cl_2 and $CFCl_3$: analysis of emissions and evidence for parent ion emission from CF_3Cl^+, **71**, 1367

CRIADO, A., BERMEJO, F.J., GARCIA-HERNÁNDEZ, M., and MARTINEZ, J.L.: Lattice dynamics of ortho-terphenyl. Implications for the current tests of mode coupling theories of the liquid-glass transition, **80**, 1263

CROSS, K.J., *see* Norman, J.B.

CUESTA, J.A., *see* Ferrero, F.S.

CUISENIER, M., *see* Lechuga-Fossat, L.

CUMMINGS, P.T., *see* Chialvo, A.A.

CUMMINGS, P.T., *see* Evans, D.J.

CUMMINGS, P.T., *see* Rudisill, E.N.

CUMMINGS, P.T., *see* Wang, B.Y.

CUMMINS, P.L., BACSKAY, G.B., and HUSH, N.S.: The effects of intermolecular interactions on the electric field gradients in ice and liquid water. The role of electrostatics, **61**, 795

CUMMINS, P.L., BACSKAY, G.B., and HUSH, N.S.: The effect of intermolecular interactions on the electric field gradients in solid ammonia, tetrazole and imidazole. The role of electrostatics, **62**, 193

CUMMINGS, P.T., *see* Lee, S.H.

CUNO, A., *see* Burden, F.R.

CURTIS, M.C., and SARRE, P.J.: Nuclear hyperfine structure in sub-Doppler electronic spectra of the Swan ($d^3\Pi_g$-$a^3\Pi_u$) system of $^{13}C_2$, **65**, 225

CUSHMAN, J.H., *see* Han, K.K.

CUSHMAN, J.H., *see* Schoen, M.

CYBULSKI, S.M., and BISHOP, D.M.: Electron-correlated calculations of magnetic properties, **76**, 1289

CYBULSKI, S.M., *see* Bishop, D.M.

CZEGLEDY, F.P., *see* Sorce, D.J.

CZUMAJ, Z.: Absorption coefficient and refractive index measurements of water in the millimetre spectra range, **69**, 787

D'AGUANNO, B., *see* Canessa, E.

D'APRANO, A., *see* Majolino, D.

D'APRANO, A., *see* Magazu, S.

DABROSKI, R., *see* Imbardelli, D.

DABROWSKI, I., HERZBERG, G., HURLEY, B.P., LIPSON, R.H., VERVLOET, M., and WANT, D.-C.: Spectra of rare gas hydrides. I. $^2\Pi$-$^2\Sigma$ and $^2\Sigma$-$^2\Sigma$ transitions of KrH and KrD, **63**, 269

DABROWSKI, I., HERZBERG, G., and LIPSON, R.H.: Spectra of rare gas hydrides. II. $^2\Pi$-$^2\Sigma$ and $^2\Sigma$-$^2\Sigma$ transitions of XeH and XeD, **63**, 289

DA COSTA, H.F.M., *see* da Silva, A.B.F.
DA COSTA, H.F.M., TRSIC, M., and MOHALLEM, J.R.: Universal gaussian and Slater-type basis sets for atoms He to Ar based on an integral version of the Hartree-Fock equations, **62**, 91
DAHM, J., MACHO, V., MARESCH, G.G., and SPIESS, H.W.: Photopolymerization study of photoresists by ESR spectroscopy and ESR imaging, **74**, 591
DAKHNOVSKII, YU. I., OVCHINNIKOV, A.A., and SEMENOV, M.B.: Low-temperature adiabatic chemical reactions in the condensed phase, **63**, 497
DALAL, N.S., *see* Rakvin, B.
DALE, M.J., *see* Jones, A.C.
DAMIANI, D., *see* Caminati, W.
DANG-NHU, M., BLANQUET, G., WALRAND, J., and DERIE, F.: Spectral intensities in the υ_3-band of $^{12}CH_3$ at 13 μm, **65**, 225
DARCY, P., *see* Jones, P.
DAS, K.K., *see* Wang, J.Z.
DA SILVA, A.B.F., DA COSTA, H.F.M., and TRSIC, M.: Universal gaussian and Slater-type bases for atoms H to Xe based on the generator coordinate Hartree-Fock method. I. Ground and certain low-lying excited states of the neutral atoms, **68**, 433
DA SILVA, A.B.F., and TRSIC, M.: Universal Gaussian and Slater-type bases for atoms H to Xe based on the generator coordinate Hartree-Fock method. II. Application of the Gaussian basis to neutral and charged diatomic molecules, **78** 1301
DASKALOPOULOU, M., and PEYERIMHOFF, S.D.: Theoretical study of the triplet states in Ar_2^{2+}, **79**, 985
DATE, R.W., HAMLEY, I.W., LUCKHURST, G.R., SEDDON, J.M., and RICHARDSON, R.M.: Orientational ordering in liquid crystals: isotope labelling neutron diffraction experiments, **76**, 951
DAUDEY, J.P., *see* Bouteiller, Y.
DAVIDENKO, N.A., *see* Kuvshinsky, N.G.
DAVIES, D.W.: An *ab initio* configuration interaction calculation for the polarizability of CsF, **63**, 1071
DAVIES, P.B., *see* Bogey, M.
DAVIES, P.B., *see* Burie, J-R.
DAVIES, P.B., and MARTIN, P.A.: Diode-laser spectroscopy of a $^3\Pi$ CO, **70**, 89
DAVIES, P.B., and DAVIS I.H.: Far infrared L.M.R. of $X^2\Pi$ NCO, **69**, 175
DAVIS, C., *see* Powles, J.G.
DAVIS, H.T., *see* Mier-y-Teran, L.
DAVIS, H.T., *see* Van Tassel, P.R.
DAVIS, H.T., *see* Zixiang Tang
DAVIS, I.H., *see* Davies, P.B.
DAVIS, S., *see* Friedrich, J.
DAVIS, S.R., *see* Andrews, L.
DAVISON, E.R., *see* Engels, B.
DAY, P., DELFS, C.D., FIGGIS, B.N., REYNOLDS, P.A., and TASSET, F.: Polarized neutron diffraction from $Cs_2KFe(CN)_6$. The orbital moment and its anisotropy,**78**, 769
DAYAN, E., DERVIL, E., LOISEL, J., PINAN-LUCARRE, J.P., and TARJUS, G.: Interaction-induced Raman and IR spectra of liquid CS_2. Temperature and perturber effects, **76**, 1457
DE ALMEIDA, W.B., and CRAW, J.S.: The molecular structure of the benzene-ClF complex, **78**, 1351
DE ALMEIDA, W.B., and HINCHLIFFE, A.: *Ab initio* vibrational spectrum of the H-bonded trimers $(HCN)_2HF$ and $HCN(HF)_2$, **69**, 305
DEBENHAM, P.M., *see* McDonald, P.J.
DE BOER, E., *see* Gribnau, M.C.M.
DE BOER, E., *see* Van der Pol, A.
DE BOER, E., *see* Wang, D.M.
DE BOER, E., *see* Willems, J.-P.
DE BROUCKÈRE, G., and BERTHIER, G.: *Ab initio* one-electron property calculations. V. Miscellaneous heterocycles and related compounds (erratum), **61**, 257
DECRESSAIN, R., ANIYREYX, J.P., CARPENTIER, L., and NAGY, J.B.: NMR in molecular crystals. An example: fluoroadamantane $C_{10}H_{15}F$, **73**, 553
DE FERAUDY, M.-F., *see* Bénière, F.M.
DEGEN, J., DIEHL, M., and SCHMIDTKE, H.-H.: Time-resolved luminescence of octahedral selenium (IV). Complexes using different excitation pulse widths, **78**, 103
DEGENHARDT, D., *see* Mager, T.

DE HAAG, P.U., SPOOREN, R., EBBEN, M., MEERTS , L. and HOUGEN, J.T.: Internal rotation in 1,4-dimethylnaphthalene studied by high resolution laser spectroscopy, **69**, 265
DEITERS, U.K.: The equation of state of soft repulsive spherical molecules, **74**, 153
DEITERS, U.K., *see* Jonah, D.A.
DEJAEGERE, A., *see* Luhmer, M.
DE KANTER, F.J.J., *see* Huis, L.
DE KOCK, B.W., *see* Polak, M.
DE LEEUW, S.W., *see* Mooij, G.C.A.M.
DE LEEUW, S.W., *see* Perram, J.W.
DE LEEUW, S.W., *see* Petersen, H.G.
DE LEEUW, S.W., *see* Smit, B.
DE LEEUW, S.W., WILLIAMS, C.P., and SMITH, B.: Evidence of phase separation in mixtures of Lennard-Jones and Stockmayer fluids, **65**, 126
DELFS, C.D., and FIGGIS, B.N.: Magnetization density in *trans*-tetraammine-dinitronickel(II), **69**, 401
DELFS, C.D., *see* Day, P.
DELGADO-BARRIO, G., *see* Gianturco, F.A.
DEL RÍO, F.: Collision frequencies and pressure in simple classical fluids, **76**, 21
DEL RÍO, F.: Effective hard-sphere diameters and equations of state, **76**, 29
DEL RÍO, F., *see* Benavides, A.H.
DEL RÍO, F., and BENAVIDES, A.L.: On some properties of the hard-sphere radial distribution function, **72**, 307
DEL RÍO, F., and GIL-VILLEGAS, A.: Collision frequencies and mean collision parameters in the Lennard-Jones system, **77**, 223
DEL RÍO, F., and LIRA, L.: Properties of the square-well fluid of variable width. I. Short-range expansion, **61**, 275
DELIKATNY, E.J., and BURNELL, E.E.: Determination of the complete order matrix of the alpha methylene segment of potassium palmitate, **67**, 757
DELIKATNY, E.J., and BURNELL, E.E.: Investigation of head group behaviour of lamellar liquid crystals. An experimental and statistical mechanical study of potassium palmitate/D_2O, **67**, 775
DE LONNGI, D.A., LONNGI, P.A., and ALEJANDRE, J.: The square-well fluid: its properties and representation. Part I: Compressibility factor, **71**, 427
DE LONNGI, D.A., and LONNGI VILLANEUVA, P.A.: Irreducible rational approximants for the hard-sphere fluid, **73**, 763
DELLA VALLE, R.G.: Local-mode to normal-mode hamiltonian transformation for X -H stretchings, **63**, 611
DELPUECH, J.-J., *see* Tekely, P.
DE LUCA, G., *see* Celebre, G.
DE LUCIA, F.C., *se* Everitt, H.O.
DE LUCIA, F.C., *see* Willey, D.R.
DEMAISON, J., *see* Graner, G.
DEMAISON, J., *see* Wlodarczak, G.
DE MIGUEL, E., and ALLEN, M.P.: Hard ellipsoids of revolution with square wells: a comparison between computer simulation and theory in the liquid-vapour region, **76**, 1275
DE MIGUEL, E., RULL, L.F., CHALAM, M.K., and GUBBINS, K.E.: Liquid-vapour coexistence of the Gay-Berne fluid by Gibbs-ensemble simulation, **71**, 1223
DE MIGUEL, E., RULL, L.F., CHALAM, M.K., GUBBINS, K.E., and VAN SWOL, F.: Location of the isotropic-nematic transition in the Gay-Berne model, **72**, 593
DE MIGUEL, E., RULL, L.F., CHALAM, M.K., and GUBBINS, K.E.: Liquid crystal phase diagram of the Gay-Berne fluid, **74**, 405
DEMCO, D.E., *see* Ursu, I.
DEMUYNCK, C., *see* Bogey, M.
DENG, Z.: Local field effect on Raman line profile of polyatomic molecules, **62**, 1003
DENLINGER, M.A., and HALL, C.K.: Molecular-dynamics simulation results for the pressure of hard-chain fluids, **71**, 541
DENNING, R.G., *see* Bartleet, J.M.
DENNINGER , G., *see* Gotschy, B.
DE PABLO, J.J., LASO, M., SIEPMANN, J.I., and SUTER, U.W.: Continuum-configurational-bias Monte Carlo simulations of long-chain alkanes, **80**, 55

DEPAEPE, J.M., RYCKAERT, J.P., and BELLEMANS, A.: Kinetics of the geometric isomerization of cyclohexene in a stochastic bath, **78**, 1575

DEPAEPE, J.-M., RYCKAERT, J.-P., PACI, E., and CICCOTTI, G.: Sampling of molecular conformations by molecular dynamics techniques, **79**, 515

DEPNER, M., SCHÜRMANN, B.L., and AURIEMMA, F.: Investigation of a poly(oxyethylene) chain by a molecular dynamics simulation in an aqueous solutions and by Langevin dynamics simulations, **74**, 715

DERIE, F., *see* Dang-Nhu, M.

DERVIL, E., *se* Dayan, E.

DE SANTIS, A., FRATTINI, R., SAMPOLI, M., MAZZACURATI, V., NARDONE, M., RICCI, M.A., and RUOCCO, G.: Raman spectra of water in the translational and librational regions. I. Study of the depolarization ratio, **61**, 1199

DE SANTIS, A., and GREGORI, A.: Induced contributions in the Rayleigh band of gaseous H_2O, **69**, 715

DE SANTIS, A., GREGORI, A., and ROCCA, D.: Simulated light-scattering experiments on liquid chlorine, **71**, 307

DE SANTIS, A., GREGORI, A., and ROCCA, D.: Nearest neighbour contributions to the atom-atom pair distribution functions of liquid iodine and chlorine, **75**, 653

DE SANTIS, A., GREGORI, A., and ROCCA, D.: Local order in liquid chlorine and the shape of $g_{a\text{-}a}(r)$ and $S(K)$, **79**, 645

DE SANTIS, A., *see* Lounila, J.

DESCAMPS, M., *see* Sauvage, J.M.

DE SMEDT, PH ., *see* Smit, B.

DESOUTER-LECOMTE, M., PAVLOV-VEREVKIN, V.B., PRAET, M. TH., CALVO, C., and LORQUET, J.C.: Statistical approximations in the study of wave packet dynamics for non-adiabatic intramolecular processes induced by a coherent excitation, **61**, 981

DE SOUZA, L.E.S., and BEN-AMOTZ, D.: Optimized perturbed hard sphere expressions for the structure and thermodynamics of Lennard-Jones fluids, **78**, 137

DESTOMBES, J.L., *see* Bogey, M.

DE SWAAN ARONS, J., *see* Cornelisse, P.M.W.

DE VIVIE, R., MARIAN, C.M., and PEYERIMHOFF, S.D.: A general procedure for the theoretical study of the Λ-doubling. Application to the $X^2\Pi$ states of OH and SH, **63**, 3

DEY, T.K., and SINHA, S.K.: Quantum corrections to equilibrium properties of molecular fluids, **73**, 427

DHAM, A.K., ALLNATT, A.R., MEATH, W.J., and AZIZ, R.A.: The Kr-Kr potential energy curve and related physical properties; the XC and HFD-B potential models, **67**, 1291

DHANARAJ, G., *see* Murthy, K.

DIANOUX, A.J., *see* Besnard, M.

DIANOUX, A.J., *see* Guillaume, F.

DÍAZ, G., *see* Acevedo, R.

DÍAZ, L.E., *see* Frydman, L.

DÍAZ, M.A., and VEGUILLAS, J.: Spectral line shapes II, **64**, 391

DÍAZ PEÑA, M., *see* Boublik, T.

DICKINSON, A.S., *see* Gianturco, F.A.

DICKINSON, A.S., and HECK, E.L.: Transport and relaxation cross-sections for He-N_2 mixtures, **70**, 239

DICKINSON, A.S., and LIU, W.-K.: Use of the classical centrifugal-sudden approximation for transport and relaxation cross-sections, **78**, 475

DICKINSON, A.S., *see* McCourt, F.R.W.

DICKINSON, A.S., *see* Liu, W.-K.

DICKINSON, A.S., *see* Wong, C.C.K.

DICKINSON, E., *see* Bujan-Nunez, M.C.

DICKINSON, E.: Monte Carlo model of competitive adsorption between interacting macromolecules and surfactants, **65**, 895

DICKINSON, E., and EUSTON, S.R.: Invited Article. Statistical study of a concentrated dispersion of deformable particles modelled as an assembly of cyclic lattice chains, **66**, 865

DICKINSON, E., and EUSTON, S.R.: Computer simulation of the competitive adsorption between polymers and small displacer molecules, **68**, 407

DICKINSON, E., and PELAN, E.G.: Molecular dynamics model of adsorbed layer at a plane fluid interface, **74**, 1115

DIEHL, M., *see* Degen, J.

DIEHL, P., *see* Jokisarri, J.

DIEHL, P., *see* Lounila, J.
DIESTLER, D.J., *see* Han, K.K.
DIESTLER, D.J., *see* Schoen, M.
DÍEZ, E., *see* Estaban, A.L.
DÍEZ, E., *see* Guilleme, J.
DÍEZ, E., SAN-FABIÁN, J., GUILLEME, J., ALTONA, C., and DONDERS, L.A.: Vicinal proton-proton coupling constants. I. Formulation of an equation including interactions between substituents, **68**, 49
DI LAURO, C., and LATTANZI, F.: On the possibility of determining ground state *K*-structure parameters from perturbed vibration-rotation spectra of symmetric-top molecules, **71**, 1303
DI LAURO, C., LATTANZI, F., and GRANER, G.: Phase conventions that render all matrix elements of the vibration-rotation Hamiltonian real, **71**, 1285
DI LAURO, C., *see* Lattanzi, F.
D'INCAN, J., *see* Bernard, A.
D'INCAN, J., *see* Effantin, C.
DIXON, R.N.: The influence of parent rotation on the dissociation dynamics of the A^1A_2'' state of ammonia, **68**, 263
DOBBS, H.T., and YEOMANS, J.M.: Capillary condensation with an array of cylinders, **80**, 877
DODD, L.R., and THEODOROU, D.N.: Analytical treatment of the volume and surface area of molecules formed by an arbitrary collection of unequal spheres intersected by planes, **72**, 1313
DODD, L.R., BOONE, T.D., and THEODOROU, D.N.: A concerted rotation algorithm for atomistic Monte Carlo simulation of polymer melts and glasses, **78**, 961
DÖGE, G., SCHNEIDER, D., and MORRESI, A.: The negative Raman non-coincidence effect of ring vibrations, **80**, 525
DOKTOROV, A.B., *see* Morozov, V.A.
DOLG, M., KÜCHLE, W., STOLL, H., PREUSS, H., and SCHWERDTFEGER, P.: *Ab initio* pseudo-potentials for Hg to Rn. II. Molecular calculations on the hydrides of HG to At and the fluorides of Rn, **74**, 1265
DOLG, M., *see* Bergner, A.
DOLG, M., *see* Häussermann, U.
DOLG, M., *see* Küchle, W.
DOMINGUEZ-ADAME, F., MÉNDEZ, MACIA, E., and GONZALEZ, M.A.: Non-local separable potentials approach to multicentre interactions, **74**, 1065
DOMKE, T.: Even/odd multiplicity editing of X-nuclei after heteronucler Hartmann-Hahn mixing, **75**, 829
DONATO, D.I., *see* Majolino, D.
DONDERS, L.A., *see* Diez, E.
DONOVAN, R.J., *see* Kvaran, Á.
DONOVAN, R.J., *see* Lawley, K.P.
DORE, J.C., *see* Farman, H.
DORE, J.C., *see* Garawi, M.
DORE, P., MORALDI, M., POLL, J.D., and BIRNBAUM, G.: Analysis of roto-translational absorption spectra induced in low density gases of non polar molecules. The methane case, **66**, 355
DORENBOS, P., *see* Andriessen, J.
DORFMÜLLER, TH., *see* Mittag, U.
DORFMÜLLER, TH., *see* Strehle, F.
DORMANN, E., *see* Lang, A.
DOUAY, M., ROGERS, S.A., and BERNATH, P.F.: Infrared Fourier transform spectroscopy of XeH, **64**, 425
DOVE, M.T.: Spontaneous strain energies associated with orientational order-disorder phase transitions, **70**, 425
DOVE, M.T., *see* Powell, B.M.
DOVE, M.T., POWELL, B.M., PAWLEY, G.S., and BARTELL, L.S.: Monoclinic phase of SF_6 and the orientational ordering transition, **65**, 353
DOVERSTÅL, M., and WEIJNITZ, P.: Lifetime measurements of the $A^3\Phi_2$, $B^3\Pi_0$, and $C^3\Delta$ $v = 0$ states of ^{48}TiO, **75**, 1357
DOVESI, R. *see* Salasco, L.
DOVESI, R., *see* Saunders, V.R.
DOVESI, R., *see* Silvi, B.

DOWNS, D.W., *see* Yenice, K.M.
DREYFUS, C., BREUILLARD, C., and GUISSANI, Y.: Rotational self-correlation function of N_2O dissolved in liquid SF_6. II. Memory function formulation analysed by molecular dynamics simulation, **62**, 1275
DROBNY, G.P., *see* Listerud, J.
DROBNY, G.P., *see* Remerowski, M.L.
DUBEY, G.S., O'SHEA, S.F., and MONSON, P.A.: Vapour-liquid equilibria for two centre Lennard-Jones diatomics and dipolar diatomics, **80**, 997
DUBINSKY, A.A., *see* Bresgunov, A. Yu.
DÜBOTZKY, A., *see* Atamny, F.
DUDDE, R., *see* Magnusson, F.O.
DUER, M.J., *see* Brown, C.A.
DUER, M.J., ESSEX, S.J., and GERLOCH, M.: A cellular ligand-field model for *l-l* spectral intensities. V. Planar and near-planar tetrachlorocopper(II) ions, **79**, 1167
DUER, M.J., ESSEX, S.J., GERLOCH, M., and JUPP, K.M.: A cellular ligand-field model for *l-l* spectral intensities. IV. Parametric structure for dynamic sources, **79**, 1147
DUMITRESCO, B., *see* Grucker, D.
DUMON, B., *see* Barreau, A.
DUMON, B., *see* Ladanyi, B.M.
DUNCAN, J.L., *see* Baggott, J.E.
DUNCAN, J.L., FERGUSON, A.M., HARPER, J., and TONGE, K.H.: ***Ab initio*** and empirical approaches to the general harmonic force field of methylene chloride, **63**, 647
DUNCAN, J.L., *see* Law, M.M.
DUNITZ, J.D., *see* Maverick, E.
DUNMUR, D.A., PALFFY-MUHORAY, P.: A mean field theory of dipole-dipole correlation in nematic liquid crystals, **76**, 1015
DUNN, L.A., *see* Fraser, K.J.
DUNNE, L.J., *see* Braga, J.P.
DUNNE, L.J., GUO, H., and MURRELL, J.N.: The role of the ***B-X*** conical intersection in the photodissociation of water, **62**, 283
DUPONT, G., MOULINASSE, S., RYCKAERT, J.P., and BAUS, M.: The b.c.c.-f.c.c-fluid triple point as obtained from Monte Carlo simulations of the Yukawa model for monodisperse colloidal suspensions, **79**, 453
DURAN, M., *see* Marti, J.
DUXBURY, G., *see* Alijah, A.
DUXBURY, G., and JUNGEN, CH.: Effects of orbital angular momentum in CH_2. The Renner-Teller effect, **63**, 981
DWORKIN, A., *see* André, D.
DYALL, K.G., *see* Brown, R.D.
DYKE, J.M., *see* Barnes, M.
DYKE, J.M., *see* Lee, E.P.F.
DYKE, J.M., *see* Wright, T.G.
DYKSTRA, C.E., *see* Augspurger, J.D.
DYMOND, J.H., and HARRIS, K.R.: The temperature and density dependence of the self-diffusion coefficient of *n*-hexadecane, **75**, 461
DYMOND, J.H., *see* Harris, K.R.
DZ-HUNG GWO, HAVENITH, M., BUSAROW, K.L., COHEN, R.C., SCHMUTTENMAER, C.A., and SAYKALLY, R.J.: Tunable far-infrared laser spectroscopy of van der Waals bonds: the $j_{k_0} = 1_0 \leftarrow 0_0\Sigma$ bending vibration of $Ar\text{-}^{14}NH_3$, **71**, 453
EASTEAL, A.J., *see* Harris, K.R.
EBBEN, M., *see* Haag, P.U.
ECHARGUI, M.A., *see* Bizot, P.
EDBERG, R., EVANS, D.J., and MORRISS, G.P.: On the nonlinear Born effect, **62**, 1357
EDWARDS, P.P., ELLABOUDY, A.S., HOLTEN, D.M., and PYPER, N.C.: The chemical dynamics of Na^- in liquid 12-crown-4 solutions deduced from ^{23}Na nuclear spin relaxation rates, **69**, 209
EDWARDS, P.P., *see* Pyper, N.C.

EFFANTIN, C., *see* Barrow, R.F.
EFFANTIN, C., *see* Bernard, A.
EFFANTIN, C., BERNARD, A., D'INCAN, J., WANNOUS, G., VERGÈS, J., and BARROW, R.F.: Studies of the electronic states of the BaF molecule. Part I: Effective constants for seven states below 30 000 cm^{-1}, **70**, 735
EFFENBERGER, F., *see* Sariciftci, N.S.
EGGEN, B.R., JOHNSTON, R.L., LI, S., and MURRELL, J.N.: Potential energy functions for atomic solids. IV. Reproducing the properties of more than one solid phase, **76**, 619
EGGENBERGER, R., GERBER, S., and HUBER, H.: The carbon dioxide dimer, **72**, 433
EGGENBERGER, R., GERBER, S., HUBER, H., SEARLES, D., and WELKER, M.: *Ab intitio* calculation of the thermal conductivity of neon in the liquid and hypercritical state over a wide pressure range, **76**, 1213
EGGENBERGER, R., GERBER, S., HUBER, H., SEARLES, D., and WELKER, M.: The use of molecular dynamics simulations with *ab initio* SCF caculations for the determination of the oxygen-17 quadrupole coupling constant in liquid water, **80**, 1177
EID, KH, M., *see* Shalabi, A.S.
EKERN, S.P., ILLIES, A.J., and MCKEE, M.L.: Theoretical study of the proton affinity of N_2O, **78**, 263
ELAND, J.H.D.: The dynamics of three-body dissociations of dications studied by the triple coincidence technique PEPIPICO, **61**, 725
ELBAYED, K., and CANET, D.: Accurate determination of interference terms between carbon-proton dipolar interactions and carbon or proton chemical shift anisotropy from longitudinal carbon-13 relaxation studies, **68**, 1033
ELBAYED, K., and CANET, D.: Behaviour of a coupled two-spin-1/2 system in the presence of a spin-locking radio-frequency field. Relaxation and Hartmann-Hahn transfers, **71**, 979
ELBAYED, K., CANET, D., and BRONDEAU, J.: Accurate determination of frequency dependent cross-relaxation terms in homonuclear and heteronuclear two spin-1/2 systems. Application to dynamic studies of aromatic moieties in micellized surfactants, **68**, 295
ELDRIDGE, M.D., MADDEN, P.A., and FRENKEL, D.: The stability of the AB_{13} crystal in a binary hard sphere system, **79**, 105
ELDRIDGE, M.D., MADDEN, P.A., and FRENKEL, D.: A computer simulation investigation into the stability of the AB_2 superlattice in a binary hard sphere system, **80**, 987
EL HACHIMI, A., *see* Bernard, A.
ELLABOUDY, A.S., *see* Edwards, P.P.
ELLINGER, Y., *see* Gillon, B.
ELLIOTT, J.R., JR., and KANETKAR, U.S.: Theory and simulation of chain-molecule fluid structure, **71**, 871
ELLIOTT, J.R., JR., KANETKAR, U.S., and VASUDEVAN, V.J.: Attractive-force effects in chain molecular fluids, **71**, 883
ELLIOTT, J.R., JR., *see* Vasudevan, V.J.
ELROD, M.J. HOST, B.C., STEYERT, D.W., and SAYKALLY, R.J.: Far-infrared vibration-rotation-tunnelling spectroscopy of ArDCl. A critical test of the H6(4,3,0) potential surface, **79**, 245
EL-SHEIKH, S.M., and TABISZ, G.C.: Perturber dependence of the collision-induced light scattering by SF_6 and CF_4, **68**, 1225
EL-SHEIKH, S.M., TABISZ, G.C., and ULIVI, L.: Three-body correlation spectra from collision-induced light scattering by SF_6 and CF_4, **72**, 345
ELWENSPOEK, M.: Solvent dependence of the step free energy on side faces of naphthalene crystals, **64**, 229
ELY, J.F., *see* Rowley, R.L.
EMERSON, A.P.J., HASHIM, R., and LUCKHURST, G.R.: Computer simulation studies of anisotropic systems. XX. On the validity of the Maier-Saupe approximations for the Gay-Berne nematogen, **76**, 241
EMSLEY, J.W., *see* Celebre, G.
EMSLEY, J.W., *see* Counsell, C.J.R.
EMSLEY, J.W., HEATON, N.J., KIMMINGS, M.K., and LONGERI, M.: The conformation and orientational order of 1-ethoxy-4-chlorobenzene dissolved in nematic liquid crystal, **61**, 433

EMSLEY, J.W., HEATON, N.J., LUCKHURST, G.R., and SHILSTONE, G.N.: Orientation order in the nematic phase of the α,ω-bis(4,4'-cyanobiphenyloxy) alkanes. A comparison between theory and experiment, **64**, 377

EMSLEY, J.W., IMRIE, C.T., LUCKHURST, G.R., and NEWMARK, R.D.: Pretransitional phenomena in liquid crystals studied via electric field induced deuterium quadrupolar splittings, **63**, 317

EMSLEY, J.W., LUCKHURST, G.R., and DACHDEV, H.S.: The orientational ordering of a biaxial solute in mixtures of nematic solvents, **67**, 151

EMSLEY, J.W., LUCKHURST, G.R., and SMITH, S.W.: The pressure and temperature dependence of the orientational order of a biaxial solute dissolved in a nematic solvent, **70**, 967

ENCISO, E., *see* Almarza, N.G.

ENCISO, E., ALMARZA, N.G., and BERMEJO, F.J.: Numerical simulation of effectively nonergodic systems, **76**, 211

ENCISO, E., *see* Alvarez, M.

ENCISO, E., *see* Bermejo, F.J.

ENCISO, E., *see* Chahid, A.

ENGDAHL, E., and MOISEYEV, N.: Perturbation analysis of gas-surface diffractive selective adsorption resonance states, **66**, 465

ENGELS, B., *see* Karna, S.P.

ENGELS, B., and PEYERIMHOFF, S.D.: The hyperfine coupling constants of the $X\ ^3\Sigma^-$ states of NH. Influence of polarization functions and configuration space on the description of spin polarization, **67**, 583

ENGELS, B., PEYERIMHOFF, S.D., and DAVIDSON, E.R.: Calculation of hyperfine coupling constants. An *ab initio* MRD-CI study for nitrogen to analyse the effects of basis sets and CI parameters, **62**, 109

ENGELS, B., *see* Staikova, M.

ENGLMAN, R., *see* Baer, M.

ENIKEEV, K.M., *see* Gaisin, N.K.

ENO, L.: Configuration dependences for crossed-beam molecular scattering in an intense laser field, **71**, 345

ENO, L.: End-point sensitivity in quantum dynamic calculations, **74**, 923

ENO, L., *see* Horn, T.R.

ENGSTRÖM, S., *see* Ahiström, P.

ERNST, M., GRIESINGER, C., ERNST, R.R., and BERMEL, W.: Optimized heteronuclear cross polarization in liquids, **74**, 219

ERNST, M., *see* Suter, D.

ERNST, R.R., *see* Ernst, M.

ERNST, R.R., *see* Griesinger, C.

ERNST, R.R., *see* Radloff, C.

ERNST, R.R., *see* Schulte-Herbrüggen, T.

ERNST, R.R., *see* Suter, D.

ERTLE, G., and HASSELBRINK, E.: Reactions at metal surfaces involving valence electron excitations, **76**, 777

ESCRIBANO, J.R., and BARRON, L.D.: Valence optical theory of vibrational circular dichroism and Raman optical activity, **65**, 327

ESPARZA, C.H., and KROMNULLER, H.: Canonical molecular dynamics simulation. A phenomenological approach, **68**, 1341

ESPINOSA-GARCIA, J.: New theoretical value of the enthalpy of formation of the OOH radical, **79**, 445

ESSEX, S.J., *see* Duer, M.J.

ESTEBAN, A.L., and GALACHE, M.P.: The r_s structure of cyclobutane from its dipolar couplings, **74**, 283

ESTEBAN, A.L., and GALACHE, M.P.: the r_α structure of oxetane as studied by NMR spectroscopy in a nematic medium, **77**, 17

ESTEBAN, A.L., GALACHE, M.P., DIEZ, E., SAN FABIAN, J., and BERMEJO, F.J.: Dependence of the dipolar couplings of tetrahydrofuran on the pseudorotation parameters, **69**, 429

ESTEBAN, A.L., *see* Galache, M.P.

ESTEBAN, A.L., *see* Guilleme, J.
ETESSE, P., CHAPMAN, W.G., and KOBAYASHI, R.: Nuclear magnetic resonance measurement of spin-lattice relaxation and self-diffusion in supercritical CO_2-*n*-hexadecane mixtures, **80**, 1145
EUSTON, S.R., *see* Dickinson, E.
EVANS, D.J.: The equivalence of Norton and Thévenin ensembles, **80**, 221
EVANS, D.J., *see* Baranyai, A.
EVANS, D.J., and BARANYAI, A.: The Gaussian thermostat, phase space compression and the conjugate pairing rule, **77**, 1209
EVANS, D.J., BARANYAI, A., and SARMAN, A.: Response theory of symmetry restricted interactions, **76**, 661
EVANS, D.J., and CUMMINGS, P.T.: Non-equilibrium molecular dynamics algorithm for the calculation of thermal diffusion in simple fluid mixtures, **72**, 893
EVANS, D.J., *see* Edberg, R.
EVANS, D.J., and HANLEY, H.J.M.: Heat induced instability in a model liquid, **68**, 97
EVANS, D.J., *see* Hood, L.M.
EVANS, D.J., LYNDEN-BELL, R.M., and MORRISS, G.P.: Steady-state structure and dynamics of a two-dimensional conducting fluid, **67**, 209
EVANS, D.J., and MORRISS, G.P.: The specific heat of non-equilibrium steady states, **61**, 1151
EVANS, D.J., and MORRISS, G.P.: Time-dependent response theory, **64**, 521
EVANS, D.J., MORRISS, G.P., and HOOD, L.M.: On the number dependence of viscosity in three dimensional fluids, **68**, 637
EVANS, D.J., and MORRISS, G.P.: Numerical test of the Kawasaki distribution function, **70**, 347
EVANS, D.J., and MURAD, S.: Thermal conductivity in molecular fluids, **68**, 1219
EVANS, D.J., *see* Murad, S.
EVANS, D.J., *see* Wang, B.Y.
EVANS, G.T.: Transport coefficients of nonspherical hard bodies: a kinetic theory approach, **74**, 775
EVANS, G.T.: Liquid crystal smectic-A phases and issues of geometry, **76**, 1359
EVANS, G.T.: Hard body models for chiral nematic liquid crystals, **77**, 969
EVANS, G.T., and MADDEN, P.A.: Vibrational energy transfer and pair dynamics in liquids: a kinetic theory study, **74**, 1171
EVANS, G.T., and SMITH, E.B.: Second virial coefficients for nonspherical molecules: a 'convex peg in a round hole' potential, **74**, 79
EVANS, G.T., *see* Samborski, A.
EVANS, G.T., *see* Tang, Shuang
EVANS, G.T., *see* Tjipto-Margo, B.
EVANS, H., *see* Cracknell, R.F.
EVANS, M.W.: Symmetry analysis of non-equilibrium time correlation functions, **67**, 1195
EVANS, M.W.: Symmetry of ensemble averages in smectic liquid crystals, **71**, 193
EVANS, M.W.: Nuclear electromagnetic resonance spectroscopy, **72**, 1195
EVANS, M.W., *see* Coffey, W.T.
EVANS, M.W., *see* Corcoran, P.M.
EVANS, M.W., and HEYES, D.M.: Correlation functions in Couette flow from group theory and molecular dynamics, **65**, 1441
EVANS, M.W., and HEYES, D.M.: Combined shear and elongational flow by non-equilibrium molecular dynamics, **69**, 241
EVANS, M.W., *see* Woźniak, S.
EVANS, R., HENDERSON, J.R., HOYLE, D.C., PARRY, A.O., and SABEUR, Z.A.: Asymptotic decay of liquid structure: oscillatory liquid-vapour density profiles and the Fisher-Widom line, **80**, 755
EVANS, R., *see* Ball, P.C.
EVANS, R., *see* Brennan, G.P.
EVANS, R., *see* Parry, A.O.
EVANS, R., *see* Telo de Gama, M.M.
EVANS, W.A.B., *see* Powles, J.G.
EVENSON, K.M., *see* Lipus, K.
EVERITT, H.O., and DE LUCIA, F.C.: The temperature dependence of fast vibrational energy transfer processes in methyl fluoride, **79**, 1087

FABER, N.M., *see* Groot, R.D.
FABRE, C., *see* André, D.
FABRE, G., *see* Bernard, A.
FABRE, D., *see* Lavorel, B.
FACELLI, J.C., *see* Solum, M.S.
FAERMAN, C.H., *see* Nyburg, S.C.
FAIN, B., *see* Alden, R.G.
FANG, J.-Y., JOHNSTON, R.L., and MCKEE, M.L.: Potential energy functions for atomic solids. V. Application to alkali metal solids, **78**, 1405
FANTONI, A.C., *see* Caminati, W.
FANTONI, R., and SNELS, M.: High resolution infrared spectrum and analysis of the υ_2 band of CF_3I, **68**, 327
FANTONI, R., and SNELS, M.: High resolution infrared spectrum and analysis of the $2\upsilon_3$, $3\upsilon_3$-υ_3 and υ_1-υ_3 bands of CF_3Br, **68**, 333
FARANTOS, S., *see* Vegiri, A.
FARANTOS, S.C., and ZACHILAS, L.: Testing molecular potential functions with bifurcation diagrams of periodic orbits, **80**, 1499
FARMAN, H., DORE, J.C., BELLISENT-FUNEL, M.-C., and MONTAGUE, D.G.: Structural studies of cyclohexane C_6D_{12} by neutron diffraction. The liquid phase, **61**, 583
FARMAN, H. O'MARA, L., DORE, J.C., and BELLISSENT-FUNEL,, M.-C.: Structural studies of cyclohexane C_6D_{12} by neutron diffraction. II. The plastic crystal phase, **73**, 855
FAVERO, L.B., *see* Caminati, W.
FEHER, M., *see* Barnes, M.
FELDER, P., *see* Frey, J.G.
FELDERHOF, B.U., *see* Cichocki, B.
FELDERHOF, B.U., *see* Kroh, H.J.
FELICI, R., *see* Caminiti, R.
FELICI, R., CILLOCO, F., and BOSI, P.: Neutron-diffraction measurements on liquid benzene, **70**, 455
FELLER, C., *see* Ingel-Mann, G.
FELLER, S.E., and MC QUARRIE, D.A.: Calculation of the force between planar electrical double layers containing counterion mixtures, **80**, 721
FELLOWS, C.E., VERGES, J., and AMIOT, C.: The NaLi electronic ground state studied by laser induced fluorescence and Fourier transform spectroscopy, **63**, 1115
FEMELAT, B., *see* Perrot, J.P.
FEMELAT, J.P., *see* Perrot, J.P.
FENRYCH, J., REYNHARDT, E.C., JURGA, S., and JURGA, K.: Molecular motions and phase changes in the perovskite-type compound $(C_{10}H_{21}NH_3)_2ZnCl_4$, **78**, 1117
FENRYCH, J., REYNHARDT, E.C., JURGA, S., and JURGA, K.: Molecular motions and phase changes in the perovskite-type compound $(C_{13}H_{27}NH_3)_2ZnCl_4$, **79**, 559
FERANCHUK, I.D., *see* An, C.Z.
FERGUSON, A.M., *see* Duncan, J.L.
FERRARINI, A., MORO, G., and NORDIO, P.L.: Conformational kinetics of aliphatic tails, **63**, 225
FERRARINI, A., MORO, G.J., NORDIO, P.L., and LUCKHURST, G.R.: A shape model for molecular ordering in nematics, **77**, 1
FERRARIO, M., MCDONALD, I.R., and SYMONS, M.C.R.: Solvent-solute hydrogen bonding in dilute solutions of CN^- and CH_3CH in water and methanol, **77**, 617
FERRARIO, M., *see* Paolini, G.V.
FERRERO, F.S., MARTINEZ-HAYA, B., PASTER, J.M. CUESTA, J.A., and TEJERO, C.F.: On one-dimensional fluids of anisotopic molecules near a hard wall, **79**, 709
FIELD, R.W., *see* Li Li
FIELD, R.W., *see* Norman, J.B.
FIGARI, G., *see* Magnasco, V.
FIGEYS, H.P., *see* Raeymaekers, P.
FIGGIS, B.N., *see* Barnes, L.A.
FIGGIS, B.N., *see* Day, P.
FIGGIS, B.N., *see* Delfs, C.D.

FIGGIS, B.N., REYNOLDS, P.A., and CABLE, J.W.: Spatial distribution of magnetization in the anisotropic $Co(H_2O)_6^{2+}$ ion from polarized neutron diffraction, **80**, 1377
FILABOZZI, A., *see* Buontempo, U.
FILABOZZI, A., and POSTORINO, P.: New determination of the He-Xe gas-gas demixing surface in the high Xe concentration region, **74**, 273
FILLAUX, F., CALILE, C.J., and KEARLEY, G.J. Rotational tunnelling and the rotational potential of methyl groups in the zinc, manganese and cobalt chloride salts of 4-methylpyridine, **80**, 671
FILSINGER, B., ZIMMERMANN, H., and HAEBERLEN, U.: ^{17}O NMR evidence for 180°-flips of $(COOH)_2$ units in dimethylmalonic acid, **76**, 157
FINN, J.E., *see* Kierlik, E.
FINN, J.E., and MONSON, P.A.: Adsorption equilibria in an isobaric ensemble, **65**, 1345
FINN, J.E., and MONSON, P.A.: Monte Carlo studies of selective adsorption on solid surfaces: adsorption from vapour mixtures, **72**, 661
FINNEY, J.L., *see* Soper, A.K.
FINNEY, J.L., *see* Turner, J.
FIRTH, N.C., *see* Jarvis, R.D.
FIRTH, N.C., KEANE, N.W., SMITH, D.J., and GRICE, R.: Reactive scattering of a supersonic fluorine atom beam : F + I_2, **66**, 1223
FIRTH, N.C., SMITH, D.J., and GRICE, R.: Reactive scattering of a supersonic fluorine atom beam: F + ICl, **61**, 859
FISCHER, J., *see* Bohn, M.
FISCHER, J., HEINBUCH, U., and WENDLAND, M.: On the hard sphere plus attractive mean field approximation for inhomogeneous fluids, **61**, 953
FISCHER, J., *see* Lotfi, A.
FISCHER, J., *see* Möller, D.
FISCHER, J., SAAGER, B., BOHN, M., OELSCHLAGER, H., and HAILE, J.M.: Specific heat of simple liquids, **62**, 1175
FISCHER, J., *see* Sokolowski, S.
FISCHER, J., *see* Vega, C.
FISCHER, J., *see* Wendland, M.
FISCHER, M.R., *see* Hoff, A.J.
FITCH, A.N., *see* Jouanneaux, A.
FITORI, P., *see* Ursu, I.
FLAD, H.-J., *see* Ingel-Mann, G.
FLAMMING, R., *see* Nguyen, M.T.
FLAUD, J.-M., *see* Camy-Peyret,
FLAUD, J.-M., *see* Lechuga-Fossat, L.
FLAUD, J.-M., *see* Perrin, A.
FLENER, P., and VESELY, F.J.: Correlated motion of two particles in a fluid. II. Molecular dynamics results, **77**, 601
FLETCHER, D.A., *see* Burghardt, I.
FLETCHER, D.A., *see* Steimle, T.C.
FLETCHER, D.A., *see* Woodward, D.R.
FLINT, C.D., *see* Acevedo, R.
FLINT, C.D., and TANNER, P.A.: Vibronic spectra of U^{4+} in octahedral crystal fields. IV. Absorption spectra and crystal field calculations, **61**, 389
FLÜGG, J., *see* Botschwina, P.
FONSECA, I.M.A., *see* Lobo, L.Q.
FORD, M.J., *see* Barnard, S.A.
FORESTER, T.R., *see* Guldbrand, L.E.
FORESTER, T.R.: A molecular dynamics study of electric field gradients in condensed B-DNA systems, **73**, 1335
FORESTER, T.R., and MCDONALD, I.R.: Molecular dynamics studies of the behaviour of water molecules and small ions in concentrated solutions of polymeric B-DNA, **72**, 643
FORMOSO, P., *see* Chidichimo, G.
FORREST, B.M., *see* Mehlig, B.

FORSMAN, H.: Dielectric relaxation of 1,2,6-hexanetriol at frequencies from 1 mHz to 10 MHz at pressures to 1 GPA, **63**, 65
FORSTER, M.J., and GILLIES, D.G.: Chemical shift anisotropy relaxation outside the extreme narrowing region. Thallium-205 N.M.R. spin relaxation of the dimethylthallium(III) cation in a viscous medium, **62**, 439
FORSTMANN, F., *see* Chen, X.S.
FORSTMANN, F., *see* Kasch, M.
FORTUNELLI, A., and SALVETTI, O.: Valence-space-only calculations on molecules: polarization effects, **75**, 1191
FOSTER, S.C., *see* Liu, X.
FOUASSIER, M., *see* Besnard, M.
FOWLER, P.W., and BUCKINGHAM, A.D.: The magnetic hyperpolarizability anisotropy of some two-electron systems, **67**, 681
FOWLER, P.W., *see* Cook, D.B.
FOWLER, P.W., *see* Kelly, H.M.
FOWLER, P.W., LAZZERETTI, P., and ZANASI, R.: Anisotropic dispersion forces in methane mixtures, **68**, 853
FOWLER, P.W., *see* Raynes, W.T.
FOWLER, P.W., and SADLEJ, A.J.: Correlated studies of electric properties of ionic molecules: alkali and alkaline-earth hydrides, halides and chalcogenides, **73**, 43
FOWLER P.W., and SADLEJ, A.J.: Long-range and overlap effects on collision-induced properties, **77**, 709
FOWLER, P.W., and STEINER, E.: Higher-order Sternheimer shieldings of the hydrogen atom, **66**, 797
FOWLER, P.W., and STEINER, E.: Electric moments and field gradients in the van der Waals H_2 system, **70**, 377
FOWLER, P.W., and STREINER, E.: Paramagnetic closed-shell molecules: the isoelectronic series CH^+, BH and BeH^-, **74**, 1147
FOWLER, P.W., TOLE, P., MUNN, R.W., and HURST, M.: Polarizability of the nitride ion in the lithium nitride crystal, **67**, 141
FOWLER, R.F., *see* Powles, J.G.
FRAHM, R., *see* Mager, T.
FRANCÉS, J.M., *see* Requena, A.
FRANCESCANGELI, O., *see* Caciuffo, R.
FRANCISCO, J.S.: Low-lying electronic states ionization potential for ethylsilylene, **65**, 1257
FRANCISCO, J.S.: Secondary dissociation pathways of ethylsilylene radical on ground and excited state potential energy surfaces, **73**, 235
FRANCISCO, J.S., *see* Gonzales, C.
FRANCISO, J.S., *see* Li, Z.
FRANCISCO, J.S., and MCDOWELL, J.J.W.: Towards the spectroscopic identification of silyvinylidene intermediate, **70**, 541
FRANCISCO, J.S., and OSTAFIN, A.: Structures of low-lying electronic states of the fluoroformyloxyl radical, **68**, 255
FRANCISCO, J.S., and WILLIAMS, I.H.: Infrared and ultraviolet spectroscopic characterization of trifluoroacetaldehyde, **76**, 1433
FRANCISCO, J.S., and ZHAO, Y.: A re-examination of the heat of formation of HO_2 using *ab initio* molecular orbital theory, **72**, 1209
FRANCISCO, J.S., *see* Zhao, Y.
FRANK, U.E., HERDEG, W., GHOSH, P.N., and HÜTTNER, W.: MW and mm wave spectra, octic-order centrifugal-distortion, ^{14}N nuclear electric quadrupole coupling, and dipole moment of the gauche tetrafluorohydrazine conformer, N_2F_4, **69**, 33
FRANK, U.E., *see* Hüttner, W.
FRANKLIN, A.M., *see* Murugesan, R.
FRANSSON, Å., and BÄCKSTRÖM, G.: Isothermal enthalpy relaxation of glassy 1,2,6-hexanetriol, **61**, 131
FRANZKE, D., VOIT, B., NUYKEN, O., and WOKAUN, A.: Pulsed ultraviolet laser photolysis of substituted phenyl azosulfonates. Wavelength dependent effects, **77**, 397

FRASER, G.T., *see* Karayakin, E.N.
FRASER, K.J., DUNN, L.A., and MORRISS, G.P.: An integral equation study of liquid acetonitrile, **61**, 775
FRATTINI, R., *see* Benassi, P.
FRATTINI, R., *see* De Santis, A.
FREEMAN, R., *see* Friedrich, J.
FREIRE, J.J., and LOPEZ RODRIGUEZ, A.: Application of the rotational isomeric model to the calculation of binary interactions between flexible chains. II. Collision integrals and viscosity coefficients of n-alkanes, **63**, 601
FREIRE, J.J., *see* Rodriguez, A.L.
FRENKEL, D., *see* Eldridge, M.D.
FRENKEL, D., *see* Hess, S.
FRENKEL, D., *see* Kranendonk, W.G.T.
FRENKEL, D.: Computer simulation of hard-core models for liquid crystals (erratum), **65**, 493
FRENKEL, D., *see* Lynden-Bell, R.M.
FRENKEL, D., *see* Mooij, G.C.A.M.
FRENKEL, D., *see* Seipmann, J.I.
FRENKEL, D., *see* Smit, B.
FRENKEL, D., and SMIT, B.: Unexpected length dependence of the solubility of chain molecules, **75**, 983
FRENKEL, D., *see* Vega, C.
FREY, J.G.: Adiabatic and diabatic approaches to bound state calculations. The Smith transformation, **65**, 1313
FREY, J.G.: Three-particle hyperspherical coordinates: permutation-inversion symmetry properties, **70**, 145
FREY, J.G.: Adiabatic and diabatic representations, coordinate and unitary transformations: coupled oscillators, **71**, 659
FREY, J.G.: Analysis of time-of-flight data. Constraints and error bars, **79**, 1287
FREY, J.G., *see* Bell, A.J.
FREY, J.G., and FELDER, P.: The analysis of anisotropic photodissociation time-of-flight data obtained from a rotating source machines, **75**, 1419
FREY, J.G., and HOLDSHIP, S.J.: Non-adiabatic corrections for coupled oscillators using Rayleigh-Schrödinger perturbation theory, **64**, 191
FREY, J.G., and HOLDSHIP, S.J.: Calculation of non-adiabatic matrix elements, **69**, 783
FREYRIA-FAVA, C., *see* Saunders, V.R.
FRIEDMAN, H.L., *see* Raineri, F.O.
FRIEDRICH, J., DAVIS, S., and FREEMAN, R.: Three-dimensional N.M.R. correlation spectroscopy with selective radiofrequency pulses, **64**, 691
FRIES, P.H., *see* Belorizky, E.
FRITZSCHE, V., *see* Knauff, O.
FROESE, R.D.J., and GODDARD, J.D.: *Ab initio* studies of the lowest singlet and triplet potential energy surfaces of CO_2, **79**, 685
FROEYEN, M., *see* Van Bell, D.
FROMMHOLD, L., *see* Borysow, J.
FROMMHOLD, L., *see* Brown, M.S.
FRONEMAN, S., *see* Reynhardt, E.C.
FRYDMAN, B., *see* Frydman, L.
FRYDMAN, L., OLIVIERI, A.C., DIAZ, L.E., FRYDMAN, B., SCHMIDT, A., and VEGA, S.: A ^{13}C solid-state NMR study of the structure and the dynamics of the polymorphs of sulphanilamide, **70**, 563
FRYE, J.M., and SEARS, T.J.: Measurement of Renner-Teller effect in $X^2\Pi$ CO_2^+ by diode laser absorption, **62**, 919
FUCHS, A.H., *see* Bénière, F.M.
FUCHS, A.H., *see* Rousseau, B.
FUCHS, R.R., *see* McCourt, F.R.W.

FUENTEALBA, P., and REYES, O.: Pseudopotential calculations on the ground state of the alkaline-earth monohydride ions, **62**, 1291
FUKASE, S., *see* Naito, S.
FUKUI K., OHYA-NISHIGUCHI H., and HIROTA N.: The relation between zero-field splittings and distortions along the normal coordinates in transition metal complexes, **71**, 126
FULLBIER, H., *see* Bengtsson, L.A.
FURER, N., *see* Stranger, R.
FURÓ, I., and HALLE, B.: Multiple quantum NMR spectroscopy on $I > 1$ nuclei in anisotropic systems, **76**, 1169
FUSHIKI, M.: A triplet correlation function for Lennard-Jones fluids, **74**, 307

GADEA, F.X., and KUNTZ, P.J.: Application of effective hamiltonian theory to the method of diatomics-in-molecules, **63**, 27
GAISIN, N.K., , MANYROV, I.R., and ENIKEEV, K.M.: Cross-correlation effects in the spin-lattice relaxation of ethanol methylene ^{13}C, **80**, 1047
GALACHE, M.P., *see* Esteban, A.L.
GALACHE, M.P., and ESTEBAN, A.L.: The structure and ring puckering vibrations of thietane from its dipolar couplings, **79**, 1137
GALLEGO, L.J., REY, C., and GRIMSON, M.J.: A Monte Carlo simulation study of the disjoining pressure in thin fluid films sterically stabilized by terminally attached chains, **74**, 383
GALLHUBER, E., *see* Braun, D.
GALLO, P., MAZZACURATI, V., and RUOCCO, G.: Evaluation of Brillouin scattering intensities from rare gas crystals. II. Introduction of short-range corrections, **71**, 97
GAMURAR, V. YA., *see* Tsukerblat, B.S.
GAN, Z.-H., and GRANT, D.M.: Pseudo-spin rotational resonance and homonuclear dipolar N.M.R. of rotating solids, **67**, 1419
GAN, Z., *see* Solum, M.S.
GANG, J., *see* Burie, J-R.
GANZMANN, I., BORGMANN, D., and WEDLER, G.: Co-adsorption of CO and O_2 on Fe. II. Calorimetric determination of heats of adsorption on polycrystalline Fe films and thermal desorption spectroscopy, **76**, 823
GAO, J., and WEINER, J.H.: Bond forces and pressure in diatomic liquids, **70**, 299
GAO, Y.-D., and HERNDON, W.C.: Tubular graphic carbon structures, **77**, 585
GARAWI, M., DORE, J.C, and CHAMPENEY, D.C.: Structural studies of liquid D-glycerol. II. Molecular conformation and long range correlations, **62**, 475
GARCIA-GUESTA, I., MIRALLES-SABATER, J., SANCHEZ-DE-MERÁS, A.M., MERCHAN, M., and NEBOT-GIL, I.: A MO-CI study on the π-coordinated interaction between palladium atom and acetylene, **66**, 659
GARCIA-GUESTA, I., SÁNCHEZ DE MERÁS, A., and NEBOT-GIL, I.: Theoretical study of acetylene- and ethylene-palladium complexes, **78**, 1449
GARCIA-HERNANDEZ, M., *see* Alvarez, M.
GARCIA-HERNANDEZ, M., *see* Chahid, A.
GARCIA-HERNANDEZ, M., *see* Criado, A.
GARCIA, N., *see* Alvarez, M.
GARCIA, N., *see* Bermejo, F.J.
GARDNER, P.J., HEYES, D.M., and PRESTON, S.R.: Molecular dynamics computer simulations of bindary Lennard-Jones fluid mixtures: Thermodynamics of mixing and transport coefficients, **73**, 141
GARROWAY, A.N., *see* Cory, D.G.
GARZÓ, V.: Generalized transport coefficients in a gas with large shear rate, **61**, 421
GARZÓ, V.: Perturbative solution of the BGK equation for very hard particle interaction, **63**, 517
GARZÓ, V.: Kinetic model for transport around uniform shear flow, **78**, 1129
GATTESCHI, D., and TSUKERBLAT, B.S.: Delocalization and exchange effects in high-nuclearity vanadium clusters, **79**, 121

GAUYACQ, D., ROCHE, A.L., SEAVER, M., COLSON, S.D., and CHUPKA, W.A.: s and d Rydberg complexes of NO probed by double-resonance multiphoton ionisation in the region $n^* = 5$ to $n^* = 25$; multichannel quantum defect analysis. Part II, **71**, 1311

GAZZILLO, D.: Direct correlation functions for negatively non-additive hard spheres in the PY approximation, **64**, 535

GAZZILLO, D.: Direct correlation functions for negatively non-additive hard spheres in the PY approximation (erratum), **68**, 1383

GEDANKEN, A., *see* Rodger, A.

GEERLINGS, P., *see* Raeymaekers, P.

GEERTSEN, J., ODDERSHEDE, J., and SABIN, J.R.: The quadrupole polarizability and spectral moments of the quadrupole oscillator strength distribution of N_2, **72**, 1267

GEERTSEN, J., *see* Sauer, S.P.A.

GEIGER, A., *see* Kneller, G.R.

GEMPERLE, C., *see* Griesinger, C.

GEORGIEV, G., *see* Zhelyaskov, V.

GERBER, S., *see* Eggenberger, R.

GERLACH, P.N., *see* Prystupa, D.A.

GERLOCH, M., *se* Bridgeman, A.J.

GERLOCH, M., *see* Brown, C.A.

GERLOCH, M., *see* Duer, M.J.

GERRAT, J., *see* Barnard, S.A.

GERRAT, J., *see* Raos, G.

GERRAT, J., *see* Sironi, M.

GERRAT, J., *see* Walters, S.G.

GERRITSEN, M., *see* Rijks, W.

GERSCHEL, A., *see* Grochulski, T.

GHAZI, F., and RIGBY, M.: The structure of hard spherocylinder fluids, **62**, 1103

GHONASGI, D., and CHAPMAN, W.G.: Theory and simulation for associating fluids with four bonding sites, **79**, 291

GHONASGI, D., and CHAPMAN, W.G.: Theory and simulation for associating chain fluids, **80**, 161

GHOSH, P.N., *see* Frank, U.E.

GIANOTTI, R.D., WANG, J., MCLAUGHLIN, I.L., and SILBERT, M.: Comments on the analytical solutions of the sticky hard rod model, **78**, 1293

GIANTURCO, F.A., DELGADO-BARRIO, G., RONCERO, O., and VILLARREAL, P.: Alternative decoupled representations for the dynamics of van der Waals molecules: a test for the He, Ne-O_2 systems, **71**, 1405

GIANTURCO, F.A., PATRIARCA, M., and RONCERO, O.: Resonant states and photodissociation cross sections in protonated rare gases. The NeH^+ and ArH^+ systems, **67**, 281

GIANTURCO, F.A., SANNA, N., and SERNA, S.: Dynamic decoupling in the calculations of transport coefficients. II. Quantum and classical results for Ne-N_2 and Ar-N_2 mixtures, **78**, 1015

GIANTURCO, F.A., SERNA, S., and SANNA, N.: Dynamical decoupling in the quantum calculations of transport coefficients. I-coupled state results for Ne-N_2 gaseous mixture, **74**, 1071

GIANTURCO, F.A., VENANZI, M., and DICKINSON, A.S.: Computed transport coefficients for van der Waals systems via realistic interactions. I. The N_2 molecule with He, Ne and Ar, **65**, 563

GIANTURCO, F.A., VENANZI, M., and DICKINSON, A.S.: Computed transport coefficients for van der Waals systems via realistic interactions. II. The O_2 molecule with He, Ne and Ar, **65**, 585

GIBSON, K.D., and SCHERAGA, H.A.: Exact calculation of the volume and surface area of fused hard-sphere molecules with unequal atomic radii, **62**, 1247

GIBSON, K.D., and SCHERAGA, H.A.: Surface area of the intersection of three spheres with unequal radii. A simplified analytical formula, **64**, 641

GILBERT, R.D., CHILD, M.S., and JOHNS, J.W.C.: Rotational analysis and assignment of the 3d ← $1b_1$ Rydberg complex in H_2O and D_2O, **74**, 473

GILLIES, D.G., *see* Forster, M.J.

GILLON, B., *see* Caciuffo, R.

GILLON, B., and ELLINGER, Y.: Theoretical spin density in nitroxides. II. The effect of alkyl substitutions on the hyperfine tensors, **63**, 967

GIORGINA, M.G., MARIANI, L., MORRESI, A., PALIANI, G., and CATALIOTTI, R.S.: Molecular dynamics and vibrational relaxations in liquid nitromethane. 1. Totally symmetric υ_1 and υ_2 modes, **75**, 1089

GILQUIN, B., *see* Ser, S.

GIL-VILLEGAS, A., *see* Del Rio, F.

GIRARD, C., and HACHE, F.: Dynamical properties of molecules physisorbed on a metal particle, **70**, 811

GIRARD, B., *see* Gouédard, G.

GIRARD, C., *see* Labani, B.

GIRARD, G., *see* Billy, N.

GIROUD-GODQUIN, A.M., *see* Carpentier, L.

GIROUD-GODQUIN, A.M., MALDIVI, P., MARCHON, J.C., BÉE, M., and CARPENTIER, L.: Alkyl chain motions of dicopper-tetraalkanoates in the crystalline and columnar phases. A quasielastic neutron scattering study, **68**, 1353

GIUNTA, G.: Hard sphere mixtures: geometrical thoughts, **67**, 1203

GIUNTA, G., *see* Caccamo, C.

GIVEN, J.A., *see* Levelt Sengers, J.M.H.

GLANDT, E.D., and KOFKE, D.A.: An efficient algorithm for the computation of pair correlation functions for hard spheres in the Percus-Yevick theory, **64**, 125

GLANDT, E.D. *see* Kofke, D.A.

GLASER, S.J., *see* Listerud, J.

GLASER, S.J., *see* Remerowski, M.L.

GLAZ, W.: On 'cross' spectral moments of the collisional polarizabilities of rigid rotors, **74**, 1019

GLINKA, C.J., *see* Hanley, H.J.M.

GOCHIN, M., PINES, A., ROSEN, M.E., RUCKER, S.P., and SCHMIDT, C.: Two-dimensional N.M.R. studies of flexible molecules in liquid crystals: orientational order and conformational probabilities of *n*-hexane, **69**, 671

GODBOLE, S.V., *see* Porwal, N.K.

GODDARD, J.D., *see* Froese, RD.J.

GODFREY, P.D., *see* Brown, R.D.

GODWIN, F.G., PATERSON, C., and GORRY, P.A.: Photofragmentation dynamics of n-C_3H_7I and i-C_3H_7I at 248 nm, **61**, 827

GOJON, E., *see* Belorizky, E.

GOLDEN, K.I., MARCH, N.H., and RAY, A.K.: Three-particle correlation function and structural theories of dense metallic liquids, **80**, 915

GOLDMAN, S.: Determination of static dielectric constant-temperature-density surfaces of a Stockmayer fluid by perturbation theory, **71**, 491

GOLDMAN, S., *see* Joslin, C.

GOLEMME, A., *see* Chidichimo, G.

GOLEMME, A., *see* Imbardelli, D.

GOLOVKO, M.F., and KRIENKE, H.: Generalized virial expansions, **68**, 967

GONZALES, C., SCHLEGEL, H.B., and FRANCISCO, J.S.: Multiple pathways for the direct formation of SiH_2 from the photodissociation of ethylsilane, **66**, 859

GONZALEZ, D.J.,*see* Canessa, E.

GONZALEZ, D.J., GONZALEZ, L.E., and SILBERT, M.: Binary Yukawa mixtures: comments on the compressibility-energy thermodynamic inconsistency in the mean spherical approximation, **71**, 157

GONZALEZ, D.J., GONZALEZ, L.E., and SILBERT, M.: Structure and thermodynamics of hard *D*-dimensional spheres: overlap volume function approach, **74**, 613

GONZALEZ, L.E., *see* Gonzalez, D.J.

GONZALEZ, M., *see* Aguilar, A.

GONZALEZ, M.A., *see* Dominguez-Adame, F.

GONZÁLEZ-LUQUE, R., MERCHÁN, M., and ROOS, B.O.: A restricted active space SCF study of the lifetime of the $A^3\Pi$ state of SH^+, **76**, 201

GONZALEZ UREÑA, A.G., *see* Verdasco, E.

GOODWIN, S.P., BOUGHEY, J.D., and HERITAGE, J.R.: Calculation of the hard sphere radial distribution function, **75**, 917
GORBATY, Y.E., *see* Bondarenko, G.V.
GORDALLA., B.C., and ZEIDLER, M.D.: NMR proton relaxation and chemical exchange in the system $H_2{}^{16}O/H_2{}^{17}O$-[$^2H_6$] dimethylsulphoxide, **74**, 975
GÖRLING, A., *see* Pyykkö, P.C
GORRY, P.A., *see* Godwin, F.
GOSCINSKA, T., *see* Harris, K.R.
GOSNEY, I., *see* Jones, A.C.
GOTSCHY, B., and DENNINGER, G.: Lineshape analysis of the ^{13}C Overhauser shift in organic conductors and semiconductors, **71**, 169
GOTSCHY, B., *see* Lang, A.
GOTZ, G., *see* Sariciftci, N.S.
GOUÉDARD, G., *see* Billy, N.
GOUÉDARD, G., BILLY, N., GIRARD, B., and VIGUÉ, J.: The IF *B-X* system. New high resolution L.I.F. spectrum and analysis, **62**, 1371
GOUÉDARD, G., BILLY, N., GIRARD, B., and VIGUÉ, J.: the IF *B-X* system. New high resolution L.I.F. spectrum and analysis (erratum), **71**, 913
GOUÉDARD, G., *see* Zalicki, P.
GOUGH, K.M., *see* Bader, R.F.W.
GOULAY, A.M., CLAIRET, F., and COHEN DE LARA, E.: Effect of electric field on internal vibration frequencies. Infrared analysis of CO_2 adsorbed in A zeolites, **73**, 845
GOULAY, A.M., *see* Cohen de Lara, E.
GOULAY, A.M., *see* Soussen-Jacob, J.
GOULDING, C.W., and RIGBY, M.: Shape effects in two-dimensional hard molecule fluids, **75**, 623
GRABEN, H.W., and RAY, J.R.: Eight physical systems of thermodynamics, statistical mechanics and computer simulations, **80**, 1183
GRAF, H.-H., KNEPPE, H., and SCHNEIDER, F.: Shear and rotational viscosity coefficients of two nematic liquid crystals, **77**, 521
GRAHAM, C.: Calculations of second light-scattering virial coefficients of linear and quasi-linear molecules, **77**, 291
GRAHAM, C., *see* Couling, V.W.
GRAHAM, C., PIERRUS, J., and RAAB, R.E.: Measurement of the electric quadrupole moments of CO_2, CO and N_2, **67**, 939
GRANER, G., DEMAISON, J., WLODARCZAK, G., ANTTILA, R., HILLMAN, J.J., and JENNINGS, D.E.: A preliminary determination of the A_0 rotational constant of propyne, **64**, 921
GRANER, G., *see* Di Lauro, C.
GRANFELDT, M., JONSSÖN, BO, and WENNERSTRÖM, H.: Electrostatic interactions in lecithin-bilayer systems. A Monte Carlo study, **64**, 129
GRANT, D.M., *see* Gan, Z.-H.
GRANT, D.M., *see* Sethi, N.K.
GRANT, D.M., *see* Solum, M.S.
GRASSI, A., *see* Baldo, M.
GRASSI, A., *see* Caniparoli, J.P.
GRAY, C.G., *see* Basile, A.G.
GRAY, C.G., *see* Joslin, C.G.
GRAY, C.G., *see* Yang, B.
GRAYCE, C.J., and HARRIS, R.A.: Electron-gas theory of the chemical shift, **71**, 1
GRAYCE, C.J., and HARRIS, R.A.: Inconsistent kinetic energy functionals of electron gases in the presence of inhomogeneous magnetic fields, **71**, 1429
GRAYCE, C.J., and HARRISON, R.A.: An electron gas calculation of the nuclear magnetic shielding tensor of $^1\Sigma_u{}^+$ H_2, **72**, 523
GRAYSON, M., *see* Raynes, W.T.
GRECI, L., *see* Caciuffo, R.
GRECI, L., *see* Maniero, A.L.
GREEN, D.V.S., *see* Young, P.

GREEN, J.C., *see* Cooper, G.
GREEN, K.A., *see* Jangkamolkulchai, A.
GREEN, K.A., and LUKS, K.D.: Robust solutions of the Yvon-Born-Green equation at very high densities. II. Long-range behaviour and solution multiplicity, **72**, 977
GREEN, N.J.B.: On the simulation of diffusion processes close to boundaries, **65**, 1399
GREEN, N.J.B., *see* Atkinson, R.A.
GREEN, N.J.B., PILLING, M.J., and CLIFFORD, P.: Approximate solution of the Debye-Smoluchowski equation for geminate ion recombination in solvents of low permittivity, **67**, 1085
GREEN, N.J.B., and PIMBLOTT, S.M.: Scavenger kinetics and the Laplace transform relationship. 1. Homogeneous systems, **74**, 795
GREEN, N.J.B., and PIMBLOTT, S.M.: Scavenger kinetics and the Laplace transform relationship. 2. Nonhomogeneous kinetics, **74**, 811
GREEN, W.H. JR, *see* Bramley, M.J.
GREEN, W.H., *see* Pinnavaia, N.
GREENFIELD, M.S., VOLD, R.L., and VOLD, R.R.: Deuterium spin relaxation and guest motion in the *n*-nonadecane/urea clathrate, **66**, 269
GREENSPAN, D.: On electron attraction, **74**, 1015
GREGORI, A., *see* De Santis, A.
GREGORY, V.P., and SCHUG, J.C.: Clustering of Lennard-Jones particles below the critical temperature, **78**, 407
GREIN, F., *see* Bruna, P.J.
GREIN, F., *see* Karna, S.P.
GRIBNAU, M.C.M., and DE BOER, E.: The magnetic structure of sodium biphenyl bistriglyme, **73**, 819
GRIBNAU, M.C.M., PIKKEMAAT, J.A., and DE BOER, E.: Magnetic properties of RbBP.2Tg, **67**, 347
GRICE, R., *see* Firth, N.C.
GRICE, R., *see* Harkin, J.J.
GRICE, R., *see* Jarvis, R.D.
GRICE, R., *see* Keane, N.W.
GRICE, R., *see* Smith, D.J.
GRICE, R., and SMITH, D.J.: Angular distributions of reactive scattering arising from persistent complexes with dissociation at arbitrary angles to the inertial axes of the transition state, **80**, 1533
GRIESINGER, C., *see* Ernst, M.
GRIESINGER, C., GEMPERLE, C., SORENSEN, O.W., and ERNST, R.R.: Symmetry in coherence transfer. Application to two-dimensional N.M.R., **62**, 295
GRIMSON, M.J.: Structure of monolayers at the air/water interface, **64**, 879
GRIMSON, M.J.: Fracture of model gel networks, **76**, 1375
GRIMSON, M.J.: Monte Carlo simulations of the melting behaviour of $A_{12}B$ Lennard-Jones heteroclusters, **77**, 797
GRIMSON, M.J.: Fracture of model gel networks under applied strain, **78**, 7
GRIMSON, M.J. and BARKER, G.C.: Model suspension of deformable particles, **71**, 635
GRIMSON, M.J., *see* Barker, G.C.
GRIMSON, M.J., *see* Canessa, E.
GRIMSON, M.J., *see* Gallego, L.J.
GRIMSON, M.J., and SILBERT, M.: A self-consistent theory of the effective interactions in charge-stabilized colloidal dispersions, **74**, 397
GROARKE, P.J., *see* Nguyen, M.T.
GROCHULSKI, T., and GERSCHEL, A.: Distinctive high frequency spectrum of liquid methyl fluoride, **77**, 539
GROCHULSKI, T., *see* Vij, J.K.
GRONLUND, W.R., *see* Pringle, W.C.
GROOT, R.D., FABER, N.M., and VAN DER EERDEN, J.P.: Hard sphere fluids near a hard wall and a hard cylinder, **62**, 861
GROSCHE, U., *see* Knauff, O.

GRUCKER, D., STEIBEL, J., MAUSS, Y., DUMITRESCO, B., ARMSPACH, J.P., and CHAMBRON, J.: Proton nuclear magnetic resonance relaxation rates in aqueous solutions of amino acids, **70**, 903
GRUEBELE, M.: Numerical potential functions for diatomic molecules. The *f*-potentials of CF^+ and CCl^+, **69**, 465
GRUEBELE, M., *see* Polak, M.
GRUNDKE, V., and BODDENBERG, B.: One and two component adsorption layers of n-hexane and benzene on graphite studied by ^2H NMR spectroscopy, **79**, 1215
GRUPP, A., *see* Rautter, J.
GRUPP, A., *see* Sariciftci, N.S.
GUARDIA, E., *see* Padró, J.A.
GUBBINS, K., *see* Chan, K.-Y.
GUBBINS, K., *see* Chapman, W.G.
GUBBINS, K., *see* Cooney, W.R.
GUBBINS, K., *see* De Miguel, E.
GUBBINS, K., *see* Heffelfinger, G.S.
GUBBINS, K., *see* Jackson, G.
GUBBINS, K., *see* Johnson, J.K.
GUBBINS, K., *see* Joslin, C.G.
GUBBINS, K., *see* Müller, E.A.
GUBBINS, K., *see* Petersen, B.
GUBBINS, K., *see* Shaoyi Jiang
GUBBINS, K., *see* Shing, K.S.
GUBBINS, K., *see* Tan, Z.
GUBBINS, K., *see* Tanaka, H.
GUBBINS, K., *see* Vega, C.
GUBBINS, K., *see* Walsh, J.M.
GÜDEL, H., *see* Stranger, R.
GUELACHVILI, G., *see* Lattanzi, F.
GUELACHVILI, G., *see* Najib, H.
GUELACHVILI, G., *see* Ouahman, M.
GÜÉMEZ, J., *see* Hernández, A.C.
GÜÉMEZ, J., *see* Velasco, S.
GUENGANT, L., *see* Vidal, D.
GUENSTER, ST., *see* Mittag, U.
GUEST, M.F., *see* Hirst, D.M.
GUIDELLI, R., *see* Boudh-Hir, M.-E.
GUILLAUME, F., CODDENS, G., DIANOUX, A.J., PETRY, W., REY-LAFON, M., and SOURISSEAU, C.: Molecular motions of decylammonium chains in the perovskite type layered compound $(C_{10}H_{21}NH_3)_2MnCl_4$. An incoherent neutron scattering study, **67**, 665
GUILLAUME, F., YARWOOD, J., and PRICE, A.H.: Infrared, Raman and microwave studies of the molecular dynamics and interactions in liquid benzonitrile, **62**, 1307
GUILLEME, J., *see* Diez, E.
GUILLEME, J., SAN-FABIÁN, J., DÍEZ, E., BERMEJO, F., and ESTABAN, A.L.: Vicinal proton-proton coupling constants. II. Analysis of the effect of interaction between geminal substituents upon vicinal couplings to methyl groups, **68**, 65
GUILLOT, B., and GUISSANI, Y.: Temperature dependence of the solubility of non-polar gases in liquids, **79**, 53
GUILLOT, B., MOUNTAIN, R.D., and BIRNBAUM, G.: Theoretical study of the three-body absorption spectrum in pure rare gas fluids, **64**, 747
GUILLOT, B., MARTEAU, PH., and OBRIOT, J.: Far-infrared absorption in nitrogen-rare gas compressed mixtures: An experimental and theoretical survey, **65**, 765
GUILYAROVSKI, A.V., *see* Ovsiannikov, V.D.
GUINET, Y., SAUVAJOL, J.L., and MULLER, M.: Raman studies of orientational disorder in crystals. The 1.fluoroadamantane plastic phase, **65**, 723
GUISSANI, Y., *see* Dreyfus, C.
GUISSANI, Y., *see* Guillot, B.

GULDBRAND, L.: The distribution and dynamics of small ions in simulations of ordered polyelectrolyte solutions, **67**, 217
GULDBRAND, L.E., FORESTER, T.R., and LYNDEN-BELL, R.M.: Distribution and dynamics of mobile ions in systems of ordered B-DNA, **67**, 473
GULDBRAND, L., *see* Nilsson, L.G.
GULLIDGE, P.N.M. *see* Powell, D.H.
GUNDU RAO, T.K., *see* Ravi Kumar, R.
GÜNTHER, E., BLÜMICH, B., and SPIESS, H.W.: Deuteron double-quantum NMR imaging of molecular order and mobility in solid polymers, **71**, 477
GUO, H.: The *B*-state photodissociation of water. A classical trajectory study, **68**, 249
GUO, H., *see* Braga, J.P.
GUO, H., *see* Dunne, L.J.
GUO, H., and MURRELL, J.N.: Dynamics of the *A*-state photodissociation of H_2O at 193 nm, **65**, 821
GUPTA, D., and HIRTZEL, C.S.: Monte Carlo studies of reactive desorption from mixed adlayers, **68**, 583
GUPTA, S.: Computer simulation and perturbation theory of fluids modelled using three- and six-site Lennard-Jones potentials, **68**, 699
GUPTA, S., and MCLAUGHLIN, E.: Conformational equation of state for fluids of chain molecules, **70**, 433
GUPTA, S., *see* Sediawan, W.B.
GUPTA, S., SEDIAWAN, W.B., and MCLAUGHLIN, E.: Computer simulation of benzene using the modified gaussian overlap and six-site potentials, **65**, 961
GURSKII, Z., HANNONGBUA, S., and HEINZINGER, K.: On the structure of concentrated lithium-liquid ammonia solutions. A molecular dynamics study, **78**, 461
GUSTAFSSON, G., and SCULLMAN, R.: Rotational analysis of the $^2\Delta_{3/2}$-$X^2\Delta_{3/2}$ and $^2\Phi_{7/2}$-$X^2\Delta_{5/2}$ sub systems of PtD, **67**, 981
GUSTAFSSON, S., and HALLE, B. Group theoretical analysis of nuclear spin relaxatin in liquid crystals and molecular solids, **80**, 549
GUSTAVSSON, T., AMIOT, C., and VERGÈS, J.: Spectroscopic investigations of the diatomic molecule RbCs by means of laser-induced fluorescence. I. Rotational analysis of the $^1\Sigma^+$ ground state up to near dissociation, **64**, 279
GUSTAVSSON, T., AMIOT, C., and VERGÈS, J.: Spectroscopic investigations of the diatomic molecule RbCs by means of laser induced fluorescence. II. Rotational analysis of five excited elecronic states, **64**, 293
GUSTAVSSON, T., AMIOT, C., and VERGES, J.: Spectroscopic investigations of the diatomic molecule RbCs by means of laser-induced fluorescence. I. Rotational analysis of the $^1\Sigma^+$ ground state up to near dissociation (erratum), **66**, 539
GUTMAN, L., and BAER., S.: Atomic pair correlation in Lennard-Jones fluids: Analysis in terms of structural diffusion models, **73**, 715
GUTOWSKI, M., VAN DUIJNEVELDT, F.B., CHALASINSKI, G., and PIELA, L.: Proper correction for the basis set superposition error in SCF calculations of intermolecular interactions, **61**, 233
GUTOWSKI, M., and PIELA, L.: Interpretation of the Hartree-Fock interaction energy between closed-shell systems, **64**, 337
GUTWERK, D., *see* Bausenwein, T.
GWO, D.-H. *see* Robinson, R.L.

HABASAKI, J.: Molecular dynamics similation of molten Li_2CO_3 and Na_2CO_3, **69**, 115
HABASAKI, J.: Molecular-dynamics study of glass formation in the Li_2SiO_3 system, **70**, 513
HACHE, F., *see* Girard, C.
HAEBERLEN, U., *see* Bernhard, T.
HAEBERLEN, U., *see* Filsinger, G.
HAEBERLEN, U., *see* Idziak, S.
HAEKEL, J., *see* Jäger, W.
HAFSKJOLD, B., IKESHOJI, T., and RATKJE, S.K.: On the molecular mechanism of thermal diffusion in liquids, **80**, 1389
HAILE, J.M., *see* Bohn, M.

HAILE, J.M., *see* Fischer, J.
HAILE, J.M., *see* Shukla, K.P.
HAIPING, B., *see* Apperley, D.C.
HALL, C.D., JOHNSON, K.A., BURGESS, A.N., WINTERTON, N., and HOWELLS, W.S.: The structure of fluid fluoroform, chlorodifluoromethane, and dichlorodifluoromethane by neutron diffraction, **74**, 27
HALL, C.K., *see* Denlinger, M.A.
HALL, C.K., *see* Honnell, K.G.
HALL, C.K., *see* Yethiraj, A.
HALL, X.S. JOHNSON, K.A., BURGESS, A.N., WINTERTON, N., and HOWELLS., W.S.: The structure of fluid dichlorodifluoromethane. A comparison between molecular dynamics simulation and neutron diffraction results, **76**, 1061
HALLAS, E., and STERNBERG, U.: New aspects of the semiempirical theory of ^{27}Al-chemical shift and its application to glasses, **68**, 315
HALLE, B.: Nuclear spin relaxation induced by lateral diffusion on a fixed or freely rotation spheroidal surface, **61**, 963
HALLE, B., *see* Carlström, G.
HALLE, B., *see* Furó, I.
HALLE, B., *see* Gustafsson, S.
HALLE, B., *see* Linse, P.
HALLE, B., *see* Quist, P.-O.
HALLE, B., and WESTLUND, P.-O.: N.M.R. lineshapes for nuclei diffusing in magnetically heterogeneous systems, **63**, 97
HAMILTON, C.A., HEWITT, J.P., MCLAUCHLAN, K.A., and STEINER, U.E.: High resolution studies of the effects of magnetic fields on chemical reactions, **65**, 423
HAMLEY, I.W., *see* Date, R.W.
HAMLEY, I.W., LUCKHURST, G.R., and SEDDON, J.M.: The influence of molecular biaxiality on intramolecular X-ray and neutron scattering from uniaxial nematic liquid crystals, **74**, 1221
HAMMONDS, K.D., MCDONALD, I.R., and TILDESLEY, D.J.: Computational studies of the structure of carbon dioxide monolayers physisorbed on the basal plane of graphite, **70**, 175
HAMMONDS, K.D., MCDONALD, I.R., and TILDESLEY, D.J.: Computational studies of the structure of monolayers of chlorine physisorbed on the basal plane of graphite **78**, 173
HAN, K.K., CUSHMAN, J.H., and DIESTLER, D.J.: Grand canonical Monte Carlo simulations of a Stockmayer fluid in a slit micropore, **79**, 537
HANDY, C.R.: An eigenvalue moment method analysis of the $V(x) = [\omega^2/2]x^2 + \alpha x^3 + \beta x^4$ anharmonic oscillator, **76**, 1235
HANDY, N.C.: The derivation of vibration-rotation kinetic energy operators, in internal coordinates, **61**, 207
HANDY, N.C., *see* Bearpark, M.J.
HANDY, N.C., *see* Bone, R.G.A.
HANDY, N.C., *see* Bramley, M.J.
HANDY, N.C., *see* Brommer, M.
HANDY, N.C., *see* Carter, S.
HANDY, N.C., *see* Jayatilaka, D.
HANDY, N.C., *see* Laming, G.J.
HANDY, N.C., *see* Murray, C.W.
HANDY, N.C., *see* Pinnavaia, N.
HANDY, N.C., *see* Smith, C.M.
HANDY, N.C., *see* Su, M-D.
HANDY, N.C., *see* Tozer, D.J.
HANH NGOC LAM, *see* Harris, K.R.
HANLEY, H.J.M., *see* Evans, D.J.
HANLEY, H.J.M., *see* Murad, S.
HANLEY, H.J.M., STRATY, G.C., GLINKA, C.J., and HAYTER, J.B.: Low-Q neutron diffraction from supercooled D-glycerol, **62**, 1165
HANLEY, H.J.M., *see* Straty, G.C.

HANLEY, H.J.M., *see* Wielopolski, P.A.
HANNONGBUA, S., *see* Gurskii, Z.
HANRATTY, M.A., *see* Celii, F.G.
HANRATTY, M.A., *see* Rosslein, M.
HANRATTY, M.A., ROSSLEIN, M., CELII, F.G., WYTTENBACH, T., and MAIER, J.P.: The $B^2\Pi_{3/2} \leftarrow X^2\Pi_{3/2}$ laser excitation spectrum of bromocyanogen cation: A rotational analysis, **64**, 865
HANSEN, J.P., *see* Barrat, J.L.
HANSEN, J.P., *see* Biben, T.
HANSEN, J.P.,*see* Kahl, G.
HANSEN, W.N., HENDERSON, D., and ULSTRUP, J.: Charge-flow and potential shifts in electrochemical double layer emersion, **68**, 401
HANSEN, W.N., KHARKATS, Y.I., and ULSTRUP, J.: Charge flow and spatial boundary conditions for potential monitoring in double-layer emersion, **80**, 1331
HANSFORD, G.M., *see* Burie, J-R.
HANSON, E.E., *see* Wong, C.C.K.
HANSON, E.E., WONG, C.C.K., and MCCOURT, F.R.W.: On the sensitivity of thermal diffusion to the anisotropy of intermolecular interaction potentials, **78**, 199
HARADA, M., *see* Kinoshita, M.
HARKIN, J.J., JARVIS, R.D., SMITH, D.J., and GRICE, R.: Reactive scattering of a supersonic fluorine-atom beam: F + C_3H_5I, C_3H_7I, $(CH_3)_2CHI$, **71**, 323
HARKIN, J.J., SMITH, D.J., and GRICE, R.: Reactive scattering of a supersonic fluorine atom beam: F + C_3H_5I, **72**, 763
HARPER, J., *see* Duncan, J.L.
HARPER, P.G., and PFAB, J.: Fragmentation dynamics of the photo-dissociated triatomic molecule, **78**, 1337
HARRIS, K.R.: The selfdiffusion coefficient and viscosity of the hard sphere fluid revisited: a comparison with experimental data for xenon, methane, ethene and trichloromethane, **77**, 1153
HARRIS, K.R., ALEXANDER, J.J., GOSCINSKA, T., MALHOTRA, R., WOOLF, L.A., and DYMOND, J.H.: Temperature and density dependence of the self-diffusion coefficients of liquid *n*-octane and toluene, **78**, 235
HARRIS, K.R., HANH NGOC LAM, RAEDT, E., EASTEAL, A.J., PRICE, W.E., and WOOLF, L.A.: The temperature and density dependences of the self-diffusion coefficient and the shear viscosity of liquid trichloromethane, **71**, 1205
HARRIS, K.R., *see* Dymond, J.H.
HARRIS, R.A., *see* Grayce, C.J.
HARRIS, R.A., *see* Suter, D.
HARRIS, R.K., *see* Apperley, D.C.
HARRIS, R.K., and ROOT, A.: High resolution phosphorus-31 N.M.R. studies of solid phosphorus pentachloride, **66**, 993
HARRISON, K.J., *see* McEwan, K.J.
HASHIM, R., *see* Emerson, A.P.J.
HASSELBRINK, E., *see* Black, J.F.
HASSELBRINK, E., *see* Ertl, G.
HATANO, M., *see* Konami, H.
HATHERLY, P.A., *see* Creasey, J.C.
HATHORN, R.M., *see* Beckmann,P.A.
HÄRTL, W., SEGSCHNEIDER, C., VERSMOLD, H., and LINSE, P.: On the structure factor of liquid-like ordered binary mixtures of colloidal suspensions, **73**, 541
HATTON, P.D., *see* Craven, C.J.
HAUSCHILD, T., *see* Smit, B.
HÄUSSERMANN, U., DOLG, M., STOLL, H., PREUSS, H., SCHWERDTFEGER, P., and PITZER, R.M.: Accuracy of energy-adjusted quasirelativisitic *ab initio* pseudopotentials. All-electron and pseudopotential benchmark calculation for Hg, HgH and their cations, **78**, 1211
HAUTMAN, J., and KLEIN, M.L.: An Ewald summation method for planar surfaces and interfaces, **75**, 379

HAUTMAN, J., and KLEIN, M.L.: Effects of particle size fluctuations in a breathing Lennard-Jones liquid, **80**, 647
HAVENITH, M., *see* Dz-Hung Gwo
HAVENITH, M., BOHLE, W., WERNER, J., and URBAN, W.: Vibration rotational spectroscopy of excited electronic states. Faraday-L.M.R. spectroscopy of CO $a^3\pi$, **64**, 1073
HAVENITH, M., SCHNEIDER, M., BOHLE, W., and URBAN, W.: Sub-Doppler Faraday LMR Spectroscopy: first applications to NO and DBr^+, **72**, 1149
HAYASHI, S., *see* Katō, T.
HAYASHI, S., *see* Nakamura, R.
HAYMET, A.D.J., *see* Laird, B.B.
HAYMET, A.D.J., *see* Mann, M.E.
HAYTER, J.B., *see* Hanley, H.J.M.
HEAD-GORDON, M.P., *see* Brown, R.D.
HEATH, J.R., *see* Hwang, H.J.
HEATON, N.J., *see* Emsley, J.W.
HEATON, N.J., and LUCKHURST, G.R.: Pretransitional behaviour in nematogens composed of flexible molecules. A molecular field theory, **66**, 65
HECHT, L. and BARRON, L.D.: Time reversal and Hermiticity characteristics of polarizability and optical activity operators. **79**, 887
HECHT, L., and BARRON, L.D.: Optical activity operators with ill defined time reversal and Hermiticity characteristics, **80**, 601
HECHT, L., and NAFIE, L.A.: Theory of natural Raman optical activity. Part I. Complete circular polarization formalism, **72**, 441
HECK, E.L., *see* Dickinson, A.S.
HEDDERICH, H.G., *see* Walker, K.A.
HEERMANN, D.W., *see* Mehlig, B.
HEFFELFINGER, G.S., VAN SWOL, F., and GUBBINS, K.: Liquid-vapour coexistence in a cylindrical pore, **61**, 1381
HEGELUND, F., KAUPPINEN, J., and WINTHER, F.: The high resolution infrared spectrum of the ν_9, ν_6 and ν_5 bands in ketene-d_2, **61**, 261
HEIMBROOK, L.A., *see* Hsu, Y.-C.
HEINBUCH, U., *see* Fischer, J.
HEINBUCH, U., *see* Wendland, M.
HEINZINGER, K., *see* Gurskii, Z.
HEINZINGER, K., *see* Pálinkás, G.
HEINZINGER, K., *see* Trokhymchuk, A.D.
HEMMERLING, B., and VERVLOET, M.: Analysis of the electronic emission $\tilde{A}^2\Sigma^+$-$\tilde{X}^2\Pi_i$ of NCO by Fourier transform spectroscopy, **78**, 1423
HENDERSON, D., *see* Chan, K.-Y.
HENDERSON, D., *see* Hansen, W.N.
HENDERSON, D., *see* Lo, Wai Yin
HENDERSON, D., and PLISCHKE, M.: Some comments on the self-consistency of the Poisson-Boltzmann theory for inhomogeneous coulomb systems, **62**, 801
HENDERSON, D., *see* Russier, V.
HENDERSON, D.J., *see* Trokhymchuk, A.D.
HENDERSON, J.R., *see* Adams, P.
HENDERSON, J.R.: Three-dimensional critical wetting and the statistical mechanics of fluids with short-range forces, **62**, 829
HENDERSON, J.R.: A derivation of external fields that create step function density profiles at wall-fluid interfaces, **74**, 1125
HENDERSON, J.R., *see* Evans, R.
HENDERSON, J.R., and TENNYSON, J.: Very highly excited vibrational states of LiCN using a discrete variable representation, **69**, 639
HENDRIKS, E.M., *see* Smit, B.
HENDRIKS, E.M., *see* Van Leeuwen, M.E.
HENRIKSSON, U., *see* Brown, M.F.

HENRY, L., *see* Lattanzi, F.
HENSLER, G., *see* Braun, D.
HERAS, J.M., VISCIDO, L., BORGMANN, D., and WEDLER, G.: AES electron beam induced fragmentation of molecular water adsorbed on copper, **75**, 487
HERDEG, W., *see* Frank, U.E.
HERITAGE, J.R., *see* Goodwin, S.P.
HERMAN, M., *see* Abbouti Temsamani, M.
HERMAN, M., HUET, T.R., and VERVLOET, M.: Spectroscopy and vibrational couplings in the $3\nu_3$ region of acetylene, **66**, 333
HERMAN, M., and HUET, T.R.: Vibrational couplings in acetylene (Corrigendum), **70**, 545
HERMAN, M., HUET, T.R., KABBADI, YU., and VANDER AUWERA, J.: *l*-type resonances in C_2H_2, **72**, 75
HERMANN, R., *see* Törring, T.
HERNÁNDEZ, A.C., VELASCO, S., and GÜÉMEZ, J.: A quasiharmonic model calculation for non-markovian far-infrared spectra of HCl in Kr and Xe liquids, **64**, 505
HERNANDO, J.A.: Thermodynamic potentials and distribution functions. I. A general expression for the entropy, **69**, 319
HERNANDO, J.A.: Thermodynamic potentials and distribution functions. II. The HNC equation as an optimized superposition approximation, **69**, 327
HERNDON, W.C., *see* Gao, Y.-D.
HERTZNER, A.W., SCHOEN, M., and MORGNER, H.: The reaction potential in anisotropic dense fluids, **68**, 1143
HERTZNER, A.W., SCHOEN, M., and MORGNER, H.: The influence of long range electrostatic forces on static properties of a quasi-Stockmayer fluid, **73**, 1011
HERWIG, K.W., and SIMMONS, R.O.: Inelastic neutron scattering from gaseous hydrogen, **75**, 1393
HERZBERG, I., *see* Dabrowski, I.
HESS, S., FRENKEL, D., and ALLEN, M.P.: On the anisotropy of diffusion in nematic liquid crystals: test of a modified affine transformation model via molecular dynamics, **74**, 765
HESS S., *see* Osipov, M.A.
HETTEMA, H., WORMER, P.E.S., and THAKKER, A.J.: Intramolecular bond length dependence of the anisotropic dispersion coefficients for interactions of rare gas atoms with N_2, CO, Cl_2, HCl and HBr, **80**, 533
HEWITT, J.P., *see* Hamilton, C.A.
HEYES, D.M.: Cluster analysis and continuum percolation of 3D square-well phases. MC and PY solutions, **69**, 559
HEYES, D.M.: Percolation of three-dimensional square-well fluid mixtures, **77**, 29
HEYES, D.M., *see* Evans, M.W.
HEYES, D.M., *see* Gardner, P.J.
HEYES, D.M., and MELROSE, J.R.: Percolation cluster statistics of Lennard-Jones fluids, **66**, 1057
HEYES, D.M., and MELROSE, J.R.: Continuum percolation of 2D Lennard-Jones and square-well phases, **68**, 359
HEYES, D.M., and POWLES, J.G.: Information theory applied to the transport coefficients of Lennard-Jones fluids, **71**, 781
HEYES, D.M., POWLES, J.G., and MONTERO, J.C.G.: Information theory applied to the transport coefficients of Lennard-Jones fluids II, **78**, 229
HIDALGO, A., *see* Requena, A.
HILL, J.-R. SAUER, J., and AHLRICHS, R.: *Ab initio* calculations of nuclear motion corrections to the geometries of water, methanol and silanol, **73**, 335
HILLIER, I.H., *see* Young, P.
HILLMAN, J.J., *see* Graner, G.
HILLS, B.P., *see* Belton, P.S.
HILLS, B.P.: Multinuclear NMR studies of water in solutions of simple carbohydrates. I. Proton and deuterium relaxation, **72**, 1099
HILLS, B.P.: The proton exchange cross-relaxation model of water relaxation in biopolymer systems, **76**, 489

HILLS, B.P.: The proton exchange cross-relaxation model of water relaxation in biopoloymer systems. II. The sol and gel states of gelatine, **76**, 509

HILLS, B.P., BELTON, P.S., and QUANTIN V.M.: Water proton relaxation in heterogeneous systems. I. Saturated randomly packed suspensions of impenetrable particles, **78**, 893

HILLS, B.P., and SNAAR, J.E.M.: Dynamic *q* space microscopy of cellular tissue, **76**, 979

HILLS, B.P., TAKACS, S.F., and BELTON, P.S.: The effects of proteins on the proton N.M.R. transverse relaxation times of water. I. Native bovine serum albumin, **67**, 903

HILLS, B.P., TAKACS, S.F., and BELTON, P.S.: The effects of proteins on the proton N.M.R. transverse relaxation times of water, II. Protein aggregation, **67**, 919

HILLS, B.P., and QUANTIN, V.M.: Water proton relaxatin in dilute and unsaturated suspensions of non-porous particles, **79**, 77

HILLS, B.P., WRIGHT, K.M., and BELTON, P.S.: N.M.R. studies of water proton relaxation in Sephadex bead suspensions, **67**, 193

HILLS, B.P., WRIGHT, K.M., and BELTON, P.S.: Proton N.M.R. studies of chemical and diffusive exchange in carbohydrate systems, **67**, 1309

HILTUNEN, Y.: Determination of the carbon-13 shielding tensors for methyl halides and haloforms by N.M.R. in mixtures of liquid crystals, **62**, 1187

HINCHLIFFE, A., *see* De Almeida, W.B.

HIPPE, D., and PEYERIMHOFF, S.D.: Theoretical spectroscopy of copper monoxide, **76**, 293

HIROIKE, K., *see* Morita, T.

HIROTA, N., *see* Fukui, K.

HIRST, D.M., and CHILD M.S.: *Ab initio* bending potential-energy curves for Rydberg states of H_2O, **77**, 463

HIRST, D.M., GUEST, M.F., and RENDELL, A.P.: *Ab initio* potential-energy curves for the molecular ions NeH^+ and ArH^+, **77**, 279

HIRSCH, G., *see* Bhanuprakash, K.

HIRSCH, G., BUENKER, R.J., and PETRONGOLO, C.: *Ab initio* study of NO_2. Part III. Potential energy functions for the two lowest $^2A'$ states in both the diabatic and adiabatic representations, **73**,1085

HIRSCH, G., *see* Bruna, P.J.

HIRSCH, G., BUENKER, R.J., and PETRONGOLO, C.: *Ab initio* study of NO_2. Part II: Non-adiabatic coupling between the two lowest $^2A'$ states and the construction of a diabatic representation, **70**, 835

HIRSCH, G., BUENKER, R.J., and PETRONGOLO, C: On the nature of the reaction path from the $^2B_2$ stationary point of the $\tilde{X}\,^2A_1$ minimum on the lowest $^2A'$ potential energy surface of NO_2, **76**, 1261

HIRSCH, G., *see* Jensen, P.

HIRSCH, G., *see* Li, Y.

HIRSCH, G., *see* Petrongolo, C.

HIRTZEL, C.S., *see* Chen, A.

HIRTZEL, C.S., *see* Gupta, D.

HISHIKAWA, A., *see* Berg, L.-E.

HOAREAU, A., *see* Broyer, M.

HOFF, A.J., and FISCHER, M.R.: Excitation migration and trappings in homogeneous and heterogeneous lattices. Application to the light-harvesting antenna complex of photosynthetic bacteria, **78**, 79

HOFFLER, U., *see* Scheffler, K.

HOFFMAN, H., *see* Rehage, H.

HOGERVORST, W., *see* Aben, I.

HOGREVE, H.: On the stability of the singly and doubly charged beryllium trimers Be_3^+ and Be_3^{++}, **76**, 1489

HOGREVE, H., *see* Ackermann, J.

HOHEISEL, C.: Pair and singlet translational and rotational diffusion in liquid model N_2. A molecular dynamics study, **62**, 239

HOHEISEL, C.: Ne/Xe at very high pressures. A molecular dynamics study using Lennard-Jones (12-6) potentials, **62**, 385

HOHEISEL, C., *see* Vogelsang, R.

HOHM, U.: A new method for the determination of the dispersion of the second recractivity virial coefficient $b_R(\lambda)$ and its application to Ar, Kr, and CO_2, **74**, 1233

HOHM, U.: Experimental determination of the dispersion in the mean linear dipole polarizability $\alpha(\omega)$ of small hydrocarbons and evaluation of Cauchy moments between 325 nm and 633 nm, **78**, 929

HOHM, U., and KERL, K.: Temperature dependence of measured mean molecular polarizability on account of translational motion, **61**, 1295

HOHM, U., and KERL, K.: Interferometric measurements of the dipole polarizability x of molecules between 300K and 1100K. I. Monochromatic measurements at $\lambda = 632.99$ nm for the noble gases and H_2, N_2, O_2, and CH_4, **69**, 803

HOHM, U., and KERL, K.: Interferometric measurements of the dipole polarizability x of molecules between 300K and 1100K. II. A new method for measuring the dispersion of the polarizability and its application to Ar, H_2, and O_2, **69**, 819

HOLCOMB, C.D., CLANCY, P., and ZOLLWEG, J.A.: A critical study of the simulation of the liquid-vapour interface of a Lennard-Jones fluid, **78**, 437

HOLDSHIP, S.J., *see* Frey, J.G.

HOLIAN, B.L., *see* Melchionna, S.

HOLLAND, J.K., NEWNHAM, D.A., and MILLS, I.M.: Vibrational overtone spectra of mono-fluoroacetylene: a preliminary report, **70**, 319

HOLLENSTEIN, H., *see* Nencini, L.

HOLLENSTEIN, H., PICCIRILLO, S., QUACK, M., and SNELS, M.: High-resolution infrared spectrum and analysis of the υ_{11}, $A_{2u}(B_2)$ fundamental band of $^{12}C_6H_6$ and $^{13}C^{12}C_5H_6$, **71**, 759

HOLLENSTEIN, H., and QUACK, M.: High resolution FTIR spectra and analysis of the υ_1 fundamental in $^{13}CF_3$, $^{35}CF_3$ and $^{13}CF_3{}^{37}Cl$, **68**, 759

HOLMBERG, V., *see* Bengtsson, L.A.

HOLOVKO, M.F., *see* Trokhymchuk, A.D.

HOLOVKO, M.F., and KALYUZHNIJ, YU. V.: Screened potentials of the site-site ion-molecular model. The mean spherical approximation, **66**, 375

HOLOVKO, M.F., and KALYUZHNYI, YU. V.: On the application of the EXP-like approximation for the description of the site-site ion-molecular models, **68**, 1239

HOLOVKO, M.F., and KALYUZHNYI, Y.V.: On the effects of association in the statistical theory of ionic systems. Analytic solution of the PY-MSA version of the Wertheim theory, **73**, 1145

HOLOVKO, M.F., *see* Kalyuzhnyi, Yu. V.

HOLOVKO, M.F., *see* Trokhymchuk, A.D.

HOLTON, D.M., *see* Edwards, P.P.

HOLYST, R.: Exact sum rules and geometrical packing effects in the system of hard rods near a hard wall in three dimensions, **68**, 391

HOLYST, R., and PONIEWIERSKI, A.: Nemantic-wall surface tension for perfectly aligned hard linear molecules, **65**, 1081

HOLYST, R., and PONIEWIERSKI, A.: Comparative study of the nematic phase-isotropic phase transition in systems of uniaxial hard cores, **68**, 381

HOLYST, R., and PONIEWIERSKI, A.: Study of the Landau bicritical points in dense systems of hard biaxial molecules, **69**, 193

HOLYST, R., and PONIEWIERSKI, A.: Smectic-A, crystalline and columnar ordering in the system of hard parallel cylinders, **71**, 561

HONG,, S.D., YOON, B.J., and JHON, M.S.: Calculation of excess free energy from averaged acceptance ratio in Monte Carlo simulation for hard sphere and hard dumb-bell fluids, **75**, 355

HONGXING ZHANG and BALASUBRAMANIAN, K.: Spectra moments of fullerene cages, **79**, 727

HONNELL, K.G., and HALL, C.K.: Monte Carlo simulation of two-dimensional dimers between hard walls. Bulk equation of state and site-density profiles, **65**, 1281

HOOD, L.M., *see* Evans, D.J.

HOOD, L.M., EVANS, D.J., and MORRISS, G.P.: Time correlation functions in the stress ensemble, **62**, 419

HOPKIRK, A., *see* Creasey, J.C.

HORE, P.J., and HUNTER, D.A.: Theory of EPR spectra of radical pairs diffusing on a spherical surface, **75**, 1401

HORE, P.J., *see* Valyaev, V.I.

HORN, M., *see* Botschwina, P.

HORN, T.R., and ENO, L.: The sensitivity approach to the analysis of parameter dependencies in reactive collision theory, **62**, 1091
HORNEMAN, V.-M., *see* Anttila, R.
HORSEWILL, A.J., *see* Clough, S.
HORSEWILL, A.J., *see* McDonald, P.J.
HORTON, T.V., *see* Byers Brown, W.
HOSHINO, K., and YOUNG, W.H.: Structure of polystyrene colloidal solutions, **62**, 1119
HOST, B.C., *see* Elrod, M.J.
HOUGEN, J.T., *see* de Haag, P.U.
HOWARD, B.J., *see* Barrow, R.F.
HOWARD, B.J., *see* Bartlett, P.
HOWARD, B.J., *and* MCKELLAR, A.R.W.: The ν_1 band of $(NO)_2$, **78**, 55
HOWARD, B.J., *see* Randall, R.W.
HOWE, C., *see* Millar, G.J.
HOWE, M.A.: Orientational correlations in the liquid halogens, **69**, 161
HOWE, M.A., *see* Saboungi, M.-L.
HOWE, M.A., WORMALD, C.J., and NEILSON, G.W.: The structure of the molecular liquids carbon monoxide (CO) and nitric oxide (NO) as determined by neutron scattering, **66**, 847
HOWELLS, W.S., *see* Alvarez, M.
HOWELLS, W.S., *see* Bermejo, F.J.
HOWELLS, W.S., *see* Hall, C.D.
HOY, A.R., *see* Lipson, R.H.
HOYDE, D.C., KEIM, E.R., and SAYKALLY, R.J.: Velocity modulation laser spectroscopy of molecular ions. The hyperfine-resolved rovibrational spectrum of HF^+, **68**, 599
HØYE, J.S., LOMBA, E., and STELL, G.: Further investigation into the low-density behaviour of the hypernetted chain equation for ionic fluids, **75**, 1217
HØYE, J.S., LOMBA, E., and STELL, G.: Analysis of the hypernetted chain equation for ionic fluids, **79**, 523
HOYLE, D.C., *see* Evans, R.
HSU, TE-JENG, and MOU, CHUNG-YUAN: Molecular dynamics study of liquid-solid transition of dense Lennard-Jones liquids, **75**, 1329
HSU, Y.-C., KENNEDY, R.A., MILLER, T.A., HEIMBROOK, L.A., and BONDYBEY, V.E.: Perturbation of the vibrational frequencies of a molecular ion by a Ne matrix, **61**, 225
HU, W.P., *see* Wang, S.P.
HUANG, T.-H., *see* Chen, W.-H.
HUANG, Y., *see* Mason, E.A.
HUBER, H., *see* Eggenberger, R.
HUBER, H., *see* Rautter, J.
HUBER, K.P., VERVLOET, M., JUNGEN, CH., and ROCHE, A.L.: Fourier transform emission spectroscopy with supersonic jets. The $4f \rightarrow 3d$ and $4f \rightarrow 4s$ transitions of nitric oxide, **61**, 501
HUET, T.R., *see* Herman, M.
HUFNAGEL, F., *see* Vij, J.K.
HUHN, B., SIMON, U., PETRI, M., ZIMMERMANN, W., and URBAN, W.: Infrared diode-laser spectroscopy of the electronic ground state of GeD ($X^2\Pi_{1/2}$). **76**, 1029
HUHN, G., *see* Simon, U.
HUIS, L., *see* Bastiaan, E.W.
HUIS, L., DE KANTER., F.J.J., and MACLEAN, C.: Chemical shielding anisotropy of ^{13}C in CH_3CN determined by NMR spectroscopy of the dielectrically oriented molecule, **73**, 1077
HUIS, L., POUWELS, P.J.W., and MACLEAN, C.: The quadrupole coupling tensor of ^{95}Mo in mesitylene molybdenum tricarbonyl, **70**, 879
HUMMER, G., and SOUMPASIS, D.M.: An extended RISM study of simple electrolytes: pair correlations in a NaCl-SPS water model, **75**, 633
HUMMER, G., SOUMPASIS, D.M., and NEUMANN, M.: Pair correlations in an NaCl-SPC water model. Simulations versus extended RISM computations, **77**, 769
HUNT, R.D., *see* Andrews, L.
HUNTER, D.A., *see* Hore, P.J.

HUNTER, I.N., MATTHEWS, G.P., and SMITH, E.B.: Viscosities of gaseous argon-hydrogen mixtures, **66**, 887
HURLEY, B.P., *see* Dabrowski, I.
HURST, M., *see* Fowler, P.W.
HUSH, N.S., *see* Cummings, P.L.
HUSH, N.S., *see* Wong, A.T.
HÜTTNER, W., *see* Frank, U.E.
HÜTTNER, W., FRANCK, U.E., MAJER, W., MAYER, K., and SPIRKO, V.: The $\nu_2 = 1$ inversional dependence of the rotational g-tensors in $^{13}NH_3$, $^{15}NH_3$ and $^{15}ND_3$, **64**, 1233
HÜTTNER, W., MAJER, W., and KÄSTLE, H.: Ground-state rotational spectrum and spectroscopic parameters of the gauche butane conformer, **67**, 131
HÜTTNER, W., PETERSEN, J.C., and RAMSAY, D.A.: Zeeman studies of microwave-optical double resonance signals in the A^1A_2-X^1A_1 system of thioformaldehyde, **63**, 811
HWANG, H.J., VAN ORDER, A., TANAKA, K., KUO, E.W., HEATH, J.R., and SAYKALLY, R.J.: Infrared laser spectroscopy of jet-cooled carbon clusters. Structure of triplet C_6, **79**, 769

IACHELLO, F., OSS, S., and VIOLA, L.: Rotation-vibration interaction and Fermi resonances of HCCF in the vibron model, **78**, 561
IACHELLO, F., OSS, S., and VIOLA, L.: Vibrational analysis of monofluoroacetylene (HCCF) in the vibron model, **78**, 545
IBBERSON, R.M., MOZE, O., and PETRILLO, C.: High resolution neutron powder diffraction studies of the low temperature crystal structure of molecular iodine (I_2), **76**, 395
ICHIKAWA, K., *see* Kameda, Y.
ICHIKAWA, K., KAMEDA, Y. YAMAGUCHI, T., WAKITA, H., and MISAWA, M.: Neutron-diffraction investigation of the intramolecular structure of a water molecule in the liquid phase at high temperatures, **73**, 79
ICHIKAWA, K., KOTANI, S., IZUMI, M., and YAMANAKA, T.: Direct correlation between lithium cation and carboxyl anion in highly concentrated aqueous solutions, **77**, 677
IDZIAK, S.: N.M.R. study of the molecular dynamics in crystalline trichloroacetic acid, **68**, 1335
IDZIAK, S., HAEBERLEN, U., and ZIMMERMANN, H.: The configuration and the dynamics of the -CD_3 groups in methyl deuterated dimethylmalonic acid. A single crystal deuteron NMR study, **73**, 571
IEVLEVA, L.D., *see* Vetchinkin, S.I.
IGEN-MANN, G., FELLER, C., FLAD, H.-J., SAVIN, A., STOLL, H., and PREUSS, H.: Comparative study of spectroscopic properties of some indium, tin and antimony compounds, **68**, 209
IGEL-MANN, G., STOLL, H., and PREUSS, H.: Pseudopotentials for main group elements (IIIa through VIIa), **65**, 1321
IGEL-MANN, G., STOLL, H., and PREUSS, H.: Pseudopotential study of monohydrides and monoxides of main group elements K through Br, **65**, 1329
IGEL-MANN, G., STOLL, H., and PREUSS, H.: Structure and ionization potentials of clusters containing heavy elements. I. Homonuclear group V clusters up to hexamers, **80**, 325
IGEL-MANN, G., STOLL, H., and PREUSS, H.: Structure and ionization potentials of clusters containing heavy elements. II. Homonuclear group VI clusters up to hexamers, **80**, 341
IGLESIAS-SILVA, G.A., *see* Nezbeda, I.
IHM, G., and MASON, E.A.: Statistical-mechanical analytical equation of state for fluid mixtures, **71**, 109
IHM, G., SONG, Y., and MASON, E.A.: Equation of state for mixtures of non-polar molecular fluids, **75**, 897
IINUMA, K., MASON, E.A., and VIEHLAND, L.A.: Tests of approximate formulae for the calculation of ion mobility and diffusion in gas mixtures, **61**, 1131
IKAWA, S., *see* Ohba, T.
IKAWA, S., and WHALLEY, E.: Effect of pressure on the Raman depolarization ratio and the vibrational relaxation of the υ_1 mode of liquid carbon tetrachloride at 22°C and 0-1.1 kbar, **75**, 659
IKEDA, Y., *see* Konami, H.
IKESHOJI, T., *see* Hafskjold, B.

IKRAM, A., TORRIE, B.H., and POWELL, B.M.: Structures of solid deuterium bromide and deuterium iodide, **79**, 1037
ILLIES, A.J., *see* Ekern, S.P.
ILYIN, V.V., *see* Antonchenko, V. Ya.
IMBARDELLI, D., *see* Chidichimo, G.
IMBARDELLI, D., WAZYNSKA, B., GOLEMME, A., CHIDICHIMO, G., and DABROWSKI, R.: ^{2}H-NMR study of molecular order and dynamics in mixtures of 80BCAB and *n*TPCHB, **79**, 1275
IMRIE, C.T., *see* Emsley, J.W.
IMRIE, D.A., and RAAB, R.E.: A new molecular theory of field gradient induced birefringence used for measuring electric quadrupole moments, **74**, 833
INABA, A., CHIMARA, H., CLARKE, S.M., and THOMAS, R.K.: The structure and heat capacity of fluoromethane monolayers adsorbed on graphite, **72**, 109
INABA, A., MORRISON, J.A., and TELFER, J.M.: Critical wetting of graphite by krypton and xenon, **62**, 961
INGMAN, P., *see* Jokisaari, J.
INNRS, K.K., *see* Meenakshi, A.
ISLAMPOUR, R., *see* Alden, R.G.
ITURBE, J., *see* Urrecha, I.
IUNG., C., *see* Chapuisat, X.
IVANOVA, A.N., *see* Antsiferova, L.I.
IZUMI, M., *see* Ichikawa, K.

JACOBS, S.M., *see* Pringle, W.C.
JACKSON, G.: Theory of closed-loop liquid-liquid immiscibility in mixtures of molecules with directional attractive force, **72**, 1365
JACKSON, G., *see* Amos, M.D.
JACKSON, G., *see* Archer, A.L.
JACKSON, G., *see* Chapman, W.G.
JACKSON, G., CHAPMAN, W.G., and GUBBINS, K.E.: Phase equilibria of associating fluids. Spherical molecules with multiple bonding sites, **65**, 1
JACKSON, G., *see* Sear, R.P.
JACKSON, G., and VAN SWOL, F.: Perturbation theory of a model hcp solid, **65**, 161
JACOBS, P.W.M., *see* Rycerz, Z.A.
JAEGERMANN, P., PLATO, M., VON MALTZAN, B., and MÖBIUS, K.: Time-resolved EPR study of exciton hopping in porphyrin dimers in their photoexcited triplet state, **78**, 1057
JAE-KWAN SUH, *see* Soon-Chul Kim
JÄGER, W., HAEKEL, J., ANDRESEN, U., and MÄDER, H.: Two-dimensional Fourier transform spectroscopy in the microwave-radiofrequency range, **68**, 1287
JALABERT, D., ROBERT, J.B., CANET, D., and TEKELY, P.: Changes in anisotropy of quinoline molecular reorientation in the liquid state as probed by ^{13}C and ^{14}N nuclear magnetic resonance relaxation times, **79**, 673
JAMIE, I.M., *see* Carlile, C.J.
JANG, JEE HWAN, *see* Xie, Yaoming
JANGKAMOLKULCHAI, A., GREEN, K.A., and LUKS, K.E.: Robust solution of the Yvon-Born-Green equation at very high densities,
JANIK POLIKS, B., *see* Photinos, D.J.
JANS-BÜRLI, S., OLDANI, M., and BAUDER, A.: Deuterium quadrupole coupling in rotational spectra, of benzene-d_1 and three isomers of fluorobenzene-d_1, **68**, 111
JANSSEN, G.J.M., *see* Tissen, J.T.W.M.
JANSSEN, R., *see* van der Mijden, J.A.M.
JARQUE, C., NOVARO, O.,and RUIZ, M.E.: Variational and perturbational CI study of the Pd-C_2H_4 molecule, **62**, 129
JARVIS, R.D., FIRTH, N.C., SMITH, D.J., and GRICE, R.: Direct dynamics of F + CCl_3Br reactive scattering, **79**, 323

JARVIS, R.D., and GRICE, R.: Angular distributions of reactive scattering arising from persistent complexes with prolate symmetric top transition states, **65**, 1205
JARVIS, R.D., and GRICE, R.: Angular distributions of reactive scattering arising from persistent complexes with oblate symmetric top transition states, **66**, 675
JARVIS, R.D., see Harkin, J.
JARVIS, R.D., LAMING, G.J., and GRICE, R.: Angular distributions of reactive scattering arising from persistent complexes by transverse dissociation of symmetric-top transition states, **70**, 667
JARVIS, R.D., WHITE, R.W.P., ZHU, Z.Z., SMITH, D.J., and GRICE, R.: Transition state dynamics of F + ICl, C_2H_5I reactive scattering, **75**, 587
JAYASANKAR, C.K., RICHARDSON, F.S., TANNER, P.A., and REID, M.F.: Analysis and comparison of holmium $4f^{10}$ energy levels in $Cs_2NaHOCl_6$ and $CsNaHoBr_6$, **61**, 635
JAYASANKAR, C.K., *see* Tanner, P.A.
JAYATILKA, D., MASLEN, P.W., AMOS, R.D., and HANDY, N.C.: Higher analytic derivatives, III. Geometrical derivatives of the dipole and dipole polarizabilities, **75**, 271
JECH, P., *see* Pospíšil, R.
JEDRZEJEK, C., *see* Konior, J.
JEENER, J., *see* Lippens, G.
JENNINGS, D.E., *see* Graner, G.
JENSEN, P., BUENKER, R.J., HIRSCH, G., and RAI, S.N.: An *ab initio* calculation of the rotational-vibrational energies in the electronic ground state of NH_2, **70**, 443
JEUNG, G.H.: Activation of CO_2 coordinated to a Cr atom, **65**, 669
JEUNG, G.H.: Activation of CO_2 coordinated to a Ti atom, **67**, 747
JEWSBURY, P., *see* Lawley, K.
JEZOWDKI, A., *see* Andersson, O.
JHON, M.S., *see* Hong, S.D.
JOHNS, J.W.C., *see* Camy-Peyret, C.
JOHNS, J.W.C., *see* Gilbert, R.D.
JOHNSON, J.K., and GUBBINS, K.E.: Phase equilibria for associating Lennard-Jones fluids from theory and simulation, **77**, 1033
JOHNSON, J.K., ZOLLWEG, J.A., and GUBBINS, K.E.: The Lennard-Jones equation of state revisited, **78**, 591
JOHNSON, K.A., *see* Hall, C.D.
JOHNSON, M.R., *see* Clough, S.
JOHNSTON, C.J., *see* Barron, L.D.
JOHNSTON, R.L., *see* Al-Derzi, A.R.
JOHNSTON, R.L., *see* Eggen, B.R.
JOHNSTON, R.L., *see* Fang, J.-Y.
JOKISAARI, J., INGMAN, P., LOUNILA, J., PULKKINEN, O., DIEHL, P., and MUENSTER, O.: Electric field gradients exprienced by the noble gas isotopes ^{21}Ne, ^{83}Kr and ^{131}Xe in thermotropic liquid crystals, 78, **41**
JONAH, D.A., and DEITERS, U.K.: On the VDW1 mixing rules applied to conformal binary mixtures at infinite dilution. A systematic improvement, **77**, 1071
JONES, A.C., DALE, M.J., BANKS, M.R., GOSNEY, I., and LANGRIDGE-SMITH, P.R.R.: Delayed ionization of laser desorbed C_{60} molecules following 193 nm photoexcitation, **80**, 583
JONES, G.L.: Elastic constants in density-functional theory, **61**, 455
JONES, H.M., *see* Creasey, J.C.
JONES, M.T., *see* Maruo, T.
JONES, P., DARCY, P., ATTARD, G.S., JONES, W.J., and WILLIAMS, G.: Angular-dependent photoselection and anisotropy of optical absorption for photochromic molecules in glassy poly(methyl methacrylate), **67**, 1053
JONES, P.J., *see* Beattie, I.R.
JONES, W.J., *see* Jones, P.
JÖHNSON, B., *see* Ahlström, P.
JÖNSSON, BO, *see* Granfeldt, M.
JONSSON, J., and LAUNILO, O.: The $C^3\Delta$-$X^3\Delta$. $A^3\Phi$-$X^3\Delta$ and $E^3\Pi$-$X^3\Delta$ systems of TiS, **79**, 95

JORGENSEN, W.L., and BRIGGS, J.M.: Monte Carlo simulations of liquid acetonitrile with a three-site model, **63**, 547
JOSHI, Y.P., TILDESLEY, D.J., AYRES, J.S., and THOMAS, R.K.: The structure of CS_2 adsorbed on graphite, **65**, 991
JOSLIN, C.G., and GRAY, C.G.: Calculation of transport coefficients using a modified Mori formalism. II. The diffusion coefficient for a dilute gas of hard spheres, **66**, 757
JOSLIN, C.G., GRAY, C.G., CHAPMAN, W.G., and GUBBINS, K.E.: Theory and simulation of associating liquid mixtures. II. **62**, 843
JOSLIN, C.G., GRAY, C.G., MICHELS, J.P.J., and KARKHECK, J.: The bulk viscosity of a square-well fluid, **69**, 535
JOSLIN, C.G., GRAY, C.G., and SULLIVAN, D.E.: Comment on 'About an information theoretical spectral line shape proposed for the collision-induced spectroscopies', **64**, 997
JOSLIN C., and GOLDMAN, S.: Second dielectric and refractivity virial coefficients of the polarizable dipolar hard-sphere fluid, **79**, 1351
JOSLIN, C., and GOLDMAN, S.: The third dielectric and pressure virial coefficients of dipolar hard sphere fluids. II. Numerical results, **79**, 499
JOUANNEAUX, A., FITCH, A.N., and COCKCROFT, J.K.: The crystal structure of $CBrF_3$ by high resolution powder neutron diffraction, **77**, 45
JUFFER, A.H., and BERENDSEN, H.J.C.: Dynamic surface boundary conditions. A simple boundary model for molecular dynamics simulations, **79**, 623
JUG, G.: Commensurate, incommensurate and rough surface phases in lipid multi-structures under applied shear, **67**, 1117
JUMEAU, D., et ANDRÉ, D.: Étude par la méthode de Monte Carlo de la phase plastique de la quinuclidine à différentes températures, **79**, 425
JUNG, W.G., ZEIDLER, M.D., and CHIEUX, P.: A neutron diffraction study of liquid methylene chloride, **68**, 473
JUNGEN, CH., *see* Duxbury, G.
JUNGEN, CH., *see* Huber, K.P.
JUNGEN, CH., *see* Larzillierè, M.
JUNGEN, M., *see* Cossart-Magos, C.
JUN WANG, MCLAUCHLIN, I.L., and SILBERT, M.: Analytical solution of the Percus-Yevick equation for the sticky hard-sphere model in odd dimensions, **79**, 331
JUPP, K.M., *see* Duer, M.J.
JURGA, K., *see* Andrew, E.R.
JURGA, K., *see* Fenrych, J.
JURGA, K., *see* Reynhardt, E.C.
JURGA, S., *see* Fenrych, J.

KABBADJ, Y., *see* Herman, M.
KAHL, G.: Analytic representation for the pair-correlation function of a hard-sphere Yukawa system, **67**, 879
KAHL, G., and HANSEN, J.-P.: Structure and thermodynamics of dilute liquid multicomponent systems, **67**, 367
KAHN, R., *see* Cohen de Lara, E.
KAHOL, P.K., and BODEN, N.: N.M.R. solid echoes in systems of dipolar-coupled inequivalent spins-1 or dipolar-coupled inequivalent pairs of spins-1/2, **69**, 833
KAHOL, P.K., *see* Rakvin, B.
KAIZU, Y., *see* Kimura, H.
KAIZU, Y., *see* Kobayashi, H.
KAKTYZGBUHM Y.V., *see* Nezbeda, Y.
KALEDIN, L.A., and SHENYAVSKAYA, E.A.: New electronic transitions in the YF spectrum; energies of the $a^3\Delta$ and $b^3\Pi$ states, **70**, 107
KALEDIN, L.A., and SHENYAVSKAYA, E.A.: Further analyses of laser induced fluorescence and emission spectra of YF. New constants for the ground $X^1\Sigma$ state up to $v = 10$, **72**, 1205
KALPAXIS, P., and RICKAYZEN, G.: Structure of a confined fluid of hard ellipsoids, **80**, 391
KALYUZHNYI, Y.V., *see* Holovko, M.F.

KALYUZHNYI, Y.V., and HOLOVKO, M.F.: An analytical study of the effects of association in a 2-2 electrolyte solution. I. Associative mean spherical approximation, **80**, 1165
KALYUZHNYI, Y.V., NEZBEDA, I.: Analytical solution of Wertheim's OZ equation for the Smith-Nezbeda model of associated liquids, **73**, 703
KALYUZHNYI, Y.U., and STELL, G.: On the effects of association in fluids with spherically symmetric interactions. I. Cluster expansions and integral equations, **78**, 1247
KAMEDA, Y., *see* Ichikawa, K.
KAMEDA, Y., KOTANI, S., and ICHIKAWA, K.: Intermolecular structure around lithium monovalent cations and nitrogen atoms in molton $LiNO_3$, **75**, 1
KAMEL, M.A., *see* Shalabi, A.S.
KANETKAR, U.S., *see* Elliott, J.R., Jr.
KANG, E.T., NEOH, K.G., and TAN, K.L.: XPS studies of charge-transfer interactions in some pyridine: organic-acceptor complexes, **70**, 1057
KAPUY, E., and KOZMUTZA, C.: Calculations for the CH_4 molecule in the framework of the localized many-body perturbation theory, **80**, 191
KAPUY, E., *see* Kozmutza, C.
KARCH, R., *see* Kömel, C.
KARKHECK, J., *see* Joslin, C.G.
KARLSSON, F., *see* Amaha, A.
KARLSTRÖM, G., *see* Åstrand, P.-O.
KARLSTRÖM, G., *see* Wolinski, K.
KARNA, S.P., and GREIN, F.: Configuration-interaction study of low-lying valence states of BO^+, **61**, 1055
KARNA, S.P., and GREIN, F.: *Ab initio* SCF and CI studies of the electric field gradient in LiH, **69**, 661
KARNA, S.P., and GREIN, F.: Dipole moment electric field gradient, field gradient and hyperfine coupling constants of the $X^2\Pi$ state of PS: *ab initio* MRD-CI studies, **77**, 135
KARNA, S.P., GREIN, F., ENGELS, B., and PEYERIMHOFF, S.D.: *Ab initio* configuration-interaction studies of the ground state potential energy and hyperfine coupling constants of $^{35}Cl_2^-$, **69**, 549
KARPFEN, A., *see* Kofranek, M.
KARRLEIN, W., MANZ, J., MOHAN, V., SCHREIER, H.-J., and SPINDLER, T.: Local versus hyperspherical modes of formaldehyde. II. State selective evaluation of vibrationally excited stretches, **64**, 563
KARTHA, V.B., *see* Talukdar, R.
KARYAKIN, E.N., FRASER, G.T., and SUENRAM, R.D.: Microwave spectrum of the $K_a = 1 \leftarrow 0$ rotation-tunnelling band of $(D_2O)_2$, **78**, 1179
KASCH, M., CHEN, X.S., and FORSTMANN, F.: The calculation of correlation functions in fluids by a weighted density concept, **75**, 415
KÄSTLE, H., *see* Hüttner, W.
KATÔ, H., *see* Katō, T.
KATŌ, T., and KATÔ, H.: Raman band shapes and the dynamics of liquid N_2O_4, **66**, 1183
KATÔ, T., OOBATAKE, M., MACHIDA, K., and HAYASHI, S.: Molecular motion and vibrational dephasing in a model of liquid N_2O_4, **77**, 177
KATOH, M., *see* Yamazaki, T.
KATZ, J., *see* Sorce, D.J.
KAUPPINEN, J., *see* Hegelund, F.
KAWAMURA, K., *see* Adya, A.K.
KAWAMURA, K., *see* Naito, S.
KEANE, N.W., *see* Firth, N.C.
KEANE, N.W., and GRICE, R.: Processional motion of asymmetric top complexes in reactive scattering, **61**, 869
KEARLEY, G.J., *see* Fillaux, F.
KEIM, E.R., *see* Hovde, D.C.
KERL, K., *see* Hohm, U.
KEITH, T.A., *see* Bader, R.F.W.

KELLÖ, V., and SADLEJ, A.J.: Electron correltion and relativistic contributions to molecular electrical properties: dipole and quadrupole moments of cyanogen halids, **75**, 209
KELLY, H.M., and FOWLER, P.W.: Quadrupole polarizabilities of anions in crystals, **80**, 135
KELLY, S.E., *see* King, F.W.
KENNEDY, R.A., *see* Carrington, A.
KENNEDY, R.A., *see* Hsu, Y.-C.
KENNEDY, R.A., MOSS, R.E., and SADLER, I.A.: Vibrational levels of HD^+ near dissociation, **64**, 177
KENYON, A.J., MCCAFFERY, A.J., and QUINTELLA, C.M.: Fluorescence depolarization as a probe of molecular dynamics within liquid jets, **72**, 965
KENYON, A.J., MCCAFFERY, A.J., QUINTELLA, C.M., and WINKEL, J.F.: A study of molecular dynamics within liquid flows using fluorescence depolarization, **74**, 871
KERL, K., *see* Hohm, U.
KESAVAMOORTHY, R., *see* Tata, B.V.R.
KETO, J.W., *see* Borysow, J.
KHARKATS, Y.I., *see* Hansen, W.N.
KHLESKOV, V.I., *see* Oshtrakh, M.I.
KHRYAPAP, V.M., **see** Antonchenko, V. Ya.
KIELPINSKI, A.L., and MURAD, S.: The effect of molecular polarizability on the properties of fluids. I. Dilute gases, **61**, 1563
KIERLIK, E., and ROSINBERG, M.L.: Packing effects in the absoption at the liquid-solid interface. Theory and computer simulation, **68**, 867
KIERLIK, E., ROSINBERG, M., FINN, J.E., and MONSON, P.A.: Binary vapour mixtures adsorbed on a graphite surface: A comparison of mean field density functional theory with results from Monte Carlo simulations, **75**, 1435
KILIAN, H.-G., *see* Peng, W.-G.
KIM, HO SOON, *see* Xie, Yaoming
KIM, KWANG S., *see* Xie, Yaoming
KIM, S.-C.: Density functional theories for classical homogeneous systems, **73**, 1179
KIMMINGS, M.K., *see* Emsley, J.W.
KIMURA, H., *see* Kobayashi, H.
KIMURA, H., KAIZU, Y., and KOBAYASHI, H.: Magnetic circular dichroism in the charge-transfer-to-solvent excited states of iodide ion in aqueous solution, **70**, 891
KIMURA, Y. and YOSHIMURA, Y.: Solute-solute potential of mean force in simple fluids at infinite dilution, **72**, 279
KIMURA, Y., and YOSHIMURA, Y.: Solvophobic interaction in a simple associated fluid. A study on the basis of Wertheim's theory on associated fluids, **76**, 737
KING, F.W., KELLY, S.E., and KUEHNE, M.A.: Nonlinear programming approach to locally constrained variational calculations on the ground state of the helium atom, **75**, 243
KING, M.A., KUHN, R., and MAIER, J.P.: $A^2\Sigma^+ \rightarrow X^2\Pi_i$ emission spectra of the supersonically cooled cation HCP^+ and DCP^+. A vibronic analysis (erratum), **62**, 1503
KING, P.M., *see* Reynolds, C.A.
KINOSHITA, M., and HARADA, M.: Numerical solution of the HNC equation for ionic systems, **65**, 599
KINOSHITA, M., and HARADA, M.: Numerical solution of the HNC equation for fluids of non-spherical particles. An efficient method with application to dipolar hard spheres, **74**, 443
KINOSHITA, M., HARADA, M., and SHIOI, A.: Characteristics of solutions of the HNC equation applied to anion-cation systems interacting through a strong long-range Coulomb potential, **70**, 1121
KINOSHITA, M., HARADA, M., and SHIOI, A.: Singularity of the HNC equation occuring at a very high density for hard spheres, **74**, 927
KINOSHITA, M., and HARADA, M.: Numerical solution of the RHNC theory for fluids of non-spherical particles near a uniform planar wall. A study with dipolar hard spheres as an example system, **79**, 145
KINOSHITA, M., HARADA, M., and SHIOI, A.: Singularity of the HNC equation occurring at a very high density for hard spheres. II, **80**, 1253
KIRBY, A.F., *see* Berry, M.T.

KISHINEVSKY, H.M., *see* Tsukerblat, B.S.
KITTAKA, S., *see* Morishige, K.
KIVELSON, D., *see* Variyar, J.E.
KJELLANDER, R., and SARMAN, S.: A study of anisotropic pair distribution theories for Lennard-Jones fluids in narrow slits. Part I. Density profiles and surface interactions, **70**, 215
KJELLANDER, R., and SARMAN, S.: A study of anisotropic pair distribution theories for Lennard-Jones fluids in narrow slits. Part II. Pair correlations and solvation forces, **74**, 665
KLEIN, D.J., *see* Posthusta, R.D.
KLEIN, H., *see* Rodger, A.
KLEIN, M.L., *see* Ryckaert, K.P.
KLEIN, M.L., *see* Hautman, J.
KLEIN, R. *see* Canessa, E.
KLOTZ, R., *see* Banichevich A.
KLOTZ, R., *see* Matsushita, T.
KLYNNING, L., *see* Balfour, W.J.
KNAUFF, O., GROSCHE, U., BONZEL, H.P., and FRITZSCHE, V.: X-ray photoelectron diffraction of Ni(110)-2 x 1-CO p2 mg layer. Intermolecular scattering, **76**, 787
KNELLER, G.R., and GEIGER, A.: Molecular dynamics studies and neutron scattering experiments on methylene chloride. I. Structure, **68**, 487
KNELLER, G.R., and GEIGER, A.: Molecular-dynamics studies and neutron-scattering experiments on methylene chloride. Part II: Dynamics, **70**, 465
KNEPPE, H., *see* Graf, H.-H.
KNÖCKEL, H., *see* Bovensmann, H.
KNÖCKEL, H., *see* Kröckertskothen, T.
KNÖCKEL, H., LINDNER, U., and TIEMANN, E.: High resolution laser excitation spectroscopy of the B1-$X^1\Sigma^+$ transition of PbS, **61**, 351
KNÖCKEL H., RICHTER, H., SIESE, M., and TIEMANN, E.: Hyperfine structure of the lowest O_g^+ and 1_g ion pair states of I_2, **68**, 917
KNORR, K., *see* Shirazi, A.R.B.
KOBAYASHI, H., KAIZU, Y., KIMURA, H., MATSUZAWA, H., and ADACHI, H.: The lowest metal-to-bipyridine charge-transfer excited state of [Cr(2,2′-bipyridine)$(CO)_4$, **64**, 1009
KOBAYASHI, H., KAIZU, Y., MATSUZAWA, H., SEKINO, H., and TORII, Y.: Electronic transfer between ligands in the tris(2,2′-bipyridine) complexes consisting of monoanion radicals. Delocalization versus localization, **78**, 909
KOBAYASHI, H., *see* Kimura, H.
KOBAYASHI, R., *see* Etesse, P.
KOCOT, A., *see* Vij, J.K.
KOFKE, D.A.: Gibbs-Duhem integration: a new method for direct evaluation of phase coexistence by molecular simulation, **78**, 1331
KOFKE, D.A., and GLANDT, E.D.: Monte Carlo simulation of multicomponent equilibria in a semigrand canonical ensemble, **64**, 1105
KOFKE, D.A., *see* Glandt, E.D.
KOFKE, D.A., *see* Mehta, M.
KOFRANEK, M., LISCHKA, H., and KARPFEN, A.: *Ab initio* studies on structure, vibrational spectra and infrared intensities of HCN, $(HCN)_2$ and $(HCN)_3$, **61**, 1519
KOHLER, F., *see* Bohn, M.
KOHLER, F., and VAN NHU, N.:The second virial coefficients of some halogenated ethanes, **80**, 795
KOIDE, A., *see* Aziz, R.A.
KOIVUSAAR, M., *see* Anttila, R.
KOK KEAN YIM, *see* Morriss, G.P.
KOLAFA, J.: On optimization of Monte Carlo simulations, **63**, 559
KOLAFA, J.: Nebular boundary conditions in Monte Carlo simulations, **74**, 143
KOLAFA, J.: Finite size effects for liquids in cyclic boundary conditions, **75**, 577
KOLAFA, J., and NEZBEDA, I.: Monte Carlo simulations on primitive models of water and methanol, **61**, 161

KOLAFA, J., and NEZBEDA, I.: Implementation of the Dahl-Anderson-Wertheim theory for realistic water-water potentials, **66**, 87
KOLAFA, J., and NEZBEDA, I.: Primitive models of associated liquids. Equation of state, liquid-gas phase transition, and percolation threshold, **72**, 777
KOLAFA, J., *see* Nezebeda, I.
KOLAFA, J., *see* Vörtler, H.L.
KOMASA, J., *see* Paidarova, I.
KOMASA, J., and THAKKAR, A.J.: Accurate multipole moments for H_2 and D_2 including the effects of electron correlation and molecular vibration and rotation, **78**, 1039
KÖMEL, C., AHLRICHS, R., and KARCH, B.: MD simulations of liquid CCl_4 with a new pair potential, **66**, 1015
KOMKO, V.M., *see* Kuvshinskij, N.F.
KONAMI, H., IKEDA, Y., HATANO, M., and MOCHIZUKI, K.: Electronic spectra of benzo-substituted phthalocyanines, **80**, 153
KONDO, A.E., and MEATH, W.J.: On the dynamics of pulsed and continuous wave laser-molecule interactions and the effects of permanent dipoles, **74**, 113
KONDOW, T., *see* Nagata, T.
KONIOR, J.: Analytical formulation of the optimized-random-phase-approximation for a hard-core Yukawa fluid, **68**, 129
KONIOR, J., and JEDRZEJEK, C.: Monte Carlo and the WCA type perturbation theory for a hard-core with two-Yukawa-tails fluid, **63**, 655
KONRAT, R., *see* Burghardt, I.
KOPTYUG, A.V., *see* Morozov, V.A.
KORTBEEK, P.J., and SCHOUTEN, J.A.: Calculation of thermodynamic properties of dense fluid neon using statistical-mechanical perturbation theory. Part I: Method, potentials and results up to 1 GPa, **69**, 981
KORTBEEK, P.J., *see* Sun, T.F.
KORTBEEK, P.J., TEN SELDAM, C.A., and SCHOUTEN, J.A.: Calculation of thermodynamic properties of dense fluid neon using statistical-mechanical perturbation theory. Part II: Results up to 6 GPa and equations of state, **69**, 1001
KOSTJUK, S.E., *see* Kuvshinkskij, N.G.
KOTANI, S., *see* Ichikawa, K.
KOTANI, S., *see* Kameda, Y.
KOVACIK, I., *see* Voronkova, V.K.
KOWALEWSKI, J., *see* Ribbing, C.
KOZAK, A., and WILLIAMS, G.: Molecular origins of optical dichroism of glassy and mobile systems as prepared by angular-dependent photoselection, **67**, 1065
KOZAK, J.J., *see* Boulu, L.G.
KOZAK, J.J., *see* Politowicz, P.A.
KOZISEK, J., *see* Voronkova, V.K.
KOZMUTZA, C., *see* Kapuy, E.
KOZMUTZA, C., TFIRST, E., and KAPUY, E.: Calculation of the interaction energy in a localized representation for several diatomic systems, **80**, 1059
KRANENDONK, W.G.T., and FRENKEL, D.: Simulation of the adhesive-hard-sphere model, **64**, 403
KRANENDONK, W.G.T., and FRENKEL, D.: Computer simulation of solid-liquid coexistence in binary hard sphere mixtures, **72**, 679
KRANENDONK, W.G.T., and FRENKEL, D.: Free energy calculations for solid solutions by computer simulations, **72**, 699
KRANENDONK, W.G.T., and FRENKEL, D.: Thermodynamic properties of binary hard-sphere mixtures, **72**, 715
KRAUSZ, E., *see* Stranger, R.
KREMP, D., *see* Sonnenburg, J.
KRIENKE, H., *see* Golovko, M.F.
KRIENKE, H., and THAMM, R.: Generaized virial expansions II. Efficient numerical algorithms for classical ionic systems, **76**, 757
KRISHNAN, M.S. TEMME, F.P., and SANCTUARY, B.C.: Theory of pulses in nuclear quadrupole resonance spectroscopy. I. Physical picture, **78**, 1385

KRISHNAN, M.S., *see* Temme, F.P.
KRÖCKERTSKOTHEN, T., KNÖCKEL, H., and TIEMANN, E.: Molecular beam rotational spectroscopy of the $X^5\Delta$ ground state of FeO, **62**, 1031
KROH, H.J., and FELDERHOF, B.U.: The Hall effect in dilute ionic solutions, **70** , 119
KROL, M.C., and ALTONA, C.: Theoretical investigations of the nature of intramolecular interactions. IV. Transferability of non-orthogonal molecular orbitals and application to mono- and difluromethane, **72**, 375
KROL, M.C., *see* Smits, G.F.
KROMHOUT, R.A., *see* Linder, B.
KROMHOUT, R.A., and LINDER, B.: Effect of van der Waals interaction on Raman transitions. I, **62**, 689
KROMHOUT, R.A., and LINDER, B.: Effect of van der Waals intraction on Raman transitions, III, **68**, 499
KRONMULLER, H., *see* Esparza, C.H.
KRYSZEWSKI, S.: On the van der Waals interaction between an atom and a dielectric medium, **78**, 1225
KÜCHLE, W. DOLG, M., STOLL, H., and PREUSS, H.: *Ab initio* pseudopotentials for Hg through Rn. I. Parameter sets and atomic calculations, **74**, 1724
KÜCHLE, W., *see* Dolg, M.
KÜCHLE, W., *see* Bergner, A.
KUEHNE, M.A., *see* King, F.W.
KUHN, R., *see* King, M.A.
KUKOLICH, S.G., *see* Roehrig, M.A.
KUKOLICH, S.G., *see* Young, S.H.
KULAGINA, T.P., *see* Antsiferova, L.I.
KUMAR, A., and MEATH, W.J.: Dipole oscillator strength properties and dispersion energies for acetylene and benzene, **75**, 311
KÜMMERLEN, J., LEITNER, A., BRUNNER, H., AUSSENEGG, F.R., and WOKAUN, A.: Enhanced dye fluorescence over silver island films: analysis of the distance dependence, **80**, 1031
KUNTZ, P.J., *see* Gadea, F.X.
KUNTZ, P.J., *see* Polák, R.
KUNZ, W., *see* Cartailler, T.
KUO, E.W., *see* Hwang, H.J.
KURT, H., *see* Atamny, F.
KURTOVIC, Z., MARCHI, M., and CHANDLER, D.: Umbrella sampling moleculer dynamics study of the dielectric constant of water, **78**, 1155
KURTZ, J., *see* Slanina, Z.
KUSALIK, P.G.: A comparison between computer simulation and theoretical results for fluids of dipolar soft spheres, **67**, 67
KUSALIK, P.G.: On the computer simulation of highly polar fluids using large systems, **73**, 1349
KUSALIK, P.G.: Determination of the transient polarization response of a dipolar fluid, **76**, 337
KUSALIK, P.G.: The distribution of fluctuations of the total dipole moment in polar liquids, **80**, 225
KUSALIK, P.G., *see* Caillol, J.M.
KUSALIK, P.G., and PATEY, G.N.: The solution of the reference hypernetted-chain approximation for water-like models, **65**, 1105
KUVSHINKSKY, N.G., DAVIDENKO, N.A., and RESHETNYAK, V.V.: On the influence of electron localization radius in a charge-transfer complex on photogeneration efficiency of current carriers in carbazole-containing semiconductors, **69**, 933
KUVSHINSKII, N.G., KOMKO, V.M., and KOSTJUK, S.J.: Two mechanisms of sensitization of photoconductivity in carbazole-containing polymeric semiconductors by Rhodamine 6G, **73**, 805
KVARAN, A., YENCHA, A.J., LAWLEY, K.P., and DONOVAN, R.J.: Analyses of the 290-400 nm oscillatory continua due to transitions from the $E(O^+)$ ion pair state of BrCl, **75**, 197
KWIATKOWSKI, J.S., and LESZCZYNSKI, J.: *Ab initio* post-Hartree-Fock study on tautomeric stabilities of phosphine oxide, phospinous acid and their thio analogues, **76**, 475

LAAKSONEN, A., *see* Maliniak, A.
LAAKSONEN, A., and STILBS, P.: Molecular dynamics and NMR study of methane-water systems, **74**, 747
LAAKSONEN, A., WESTLUND, P.-O.: A molecular dynamics simulation of HCl. A study of the vibrational dephasing mechanism, **73**, 663
LABANI, B., GIRARD, C., and MAGHEZZI, S.: van der Waals interactions between a molecule and a small metallic sphere, **69**, 85
LABÍK, S., *see* Malijevský, A.
LABÍK, S., and MALIJEVSKÝ, A.: Bridge function for hard spheres in high density and overlap regions, **67**, 431
LABIK, S., MALIJEVSKÝ, A., POPIŠIL, R., and SMITH, W.R.: An accurate integral equation for molecular fluids, IV. Hard prolane spherocylinders, **74**, 261
LABÍK, S., MALIJEVSKÝ, A., and SMITH, W.R.: An accurate integral equation for molecular fluids. I. Hard homonuclear diatomics, **73**, 87
LABÍK, S., MALIJEVSKÝ, A., and SMITH, W.R.: An accurate integral equation for molecular fluids. II. Hard heteronuclear diatomics, **73**, 495
LABÍK, S., *see* Pospišil, R.
LABÍK, S., SMITH, W.R., and NEZBEDA, A.: The RAM perburbation theory for molecular fluid mixtures. I. Site-centred correlation functions, **62**, 775
LABÍK, S., SMITH, W.R., POSPÍSIL, R., and MALIJEVSKY, A.: Non-spherical bridge function theory of molecular fluids. I. The hard-dumbbell fluid, **69**, 649
LABIK, S., *see* Smith, W.R.
LABLANQUIE, P., *see* Stace, A.J.
LABORANTI, L.M., *see* Mognaschi, E.R.
LABRUNIE, L., *see* Bervas, H.
LADANYI, M., *see* Barreau, A.
LADANYI, B.M., BARREAU, A., and DUMON, B.: Density and tempeature dependence of spectral moments in depolarized light scattering by rare gases, **77**, 735
LADANYI, M., *see* Buchner, M.
LADO, F.: Integrals over the triplet distribution function without the triplet distribution function, **72**, 1387
LADO, F., *see* Ward, D.A.
LADO-BORODOWSKY, O., *see* Perrin, A.
LAGO, S., *see* Boublik, T.
LAGO, S., *see* López Rodriguez, A.
LAGO, S., *see* Padilla, P.
LAGO, S., *see* Vega, C.
LAIDIG, K.E., *see* Bader, R.F.W.
LAIRD, B.B., and HAYMET, A.D.J.: Phase diagram for the inverse sixth power potential system from molecular dynamics computer simulation, **75**, 71
LAKHLIFI, A.: Analysis of the interaction potential of a molecule physisorbed on NaCl(100) surface, **78**, 659
LAM, B., *see* Bishop, D.M.
LAMBERT, I.R. *see* Creasey, J.C.
LAMBERT, R.M., *see* Broomfield, K.
LAMING, G.J., HANDY, N.C., and AMOS, R.D.: Kohn-Sham calculations on open-shell diatomic molecules, **80**, 1121
LAMING, G.J., *see* Jarvis, R.D.
LAMING, G.J., *see* Murray, C.W.
LANE, S., *see* Szalay, V.
LANG, E.W., *see* Speedy, R.J.
LANG, A., NAARMANN, H., RÖSLER, G., GOTSCHY, B., WINTER, H., and DORMANN, E.: Synthesis and characterization of new multi-radical compound, 1,3,5-tri-6′-(1,3,5-triphenylverdazyl)-benzene, **79**, 1051
LANGFELDEROVA., H., *see* Boronkova, V.K.
LANGRIDGE-SMITH, P.R.R., *see* Jones, A.C.

LANGRIDGE-SMITH, P., *see* Lawley, K.
LARHER, Y., *see* Ser, S.
LARIN, A.B., and PARBUZIN, V.S.: Theoretical estimate of *ortho-para* separation coefficients for H_2 and D_2 on A-type zeolites for small and medium coverage, **77**, 869
LARSEN, S.Y., *see* Berrondo, M.
LARSEN, S.Y., and ZHEN, J.: Low energy behaviour of a three-body phase shift, **63**, 581
LARSEN, S.Y., and ZHEN, J.: The quantum mechanical third cluster for a binary step potential, **65**, 237
LARSON, A.C., *see* Torrie, B.H.
LARSSON, T.P., *see* Westlund, P.-O.
LARZILLIERÈ, M., and JUNGEN, CH.: Fast ion beam laser spectroscopy of N_2O^+. Effects of orbital angular momentum and vibrational anharmonicity, **67**, 807
LASO, M., *see* De Pablo, J.J.
LASSEGUES, J.C., *see* Besnard, M.
LASSEGUES, J.C., and CAVAGNAT, D.: Neutron scattering study of the proton dynamics in aqueous solutions of sulphuric acid and caesium sulphate, **68**, 803
LASNE, M.C., *see* Wlodarczak, G.
LATOUR, J.-M., *see* Belorizky, E.
LATTANZI, F., *see* Di Lauro, C.
LATTANZI, F., DE LAURO, C., and BÜRGER, H.: The high-resolution infrared spectrum of $H_3Si^{79}Br$ from 2100 to 2330 cm^{-1}. The υ_1 and υ_4 fundamentals, **72**, 575
LATTANZI, F., DI LAURO, C.M., and GUELACHVILI, G.: Rotational analysis and anomalous intensity patterns of the 2430 to 2770 cm^{-1} infrared spectrum of CH_3I, **66**, 509
LATTANZI, F., DI LAURO, C., HENRY, L., VALENTIN, A., and BÜRGER, H.: The high resolution Fourier transform infrared spectrum of $H_3\ ^{74}Ge^{37}Cl$ from 1000 to 2250 cm^{-1}, **65**, 85
LATTANZI, F., DI LAURO, C.M., HENRY, L., VALENTIN, A., and BÜRGER, H.: The high resolution Fourier transform infrared spectrum of $H_3\ ^{70}Ge^{35}Cl$ from 2000 to 2250 cm^{-1}, **66**, 1027
LAUNAY, F., *see* Cossart-Magos, C.
LAUNILA, O.: Spectroscopy of MnCl: vibrational analysis of a band system near 877 nm and observation of a new band system near 1001 nm, **76**, 319
LAUNILA, O., *see* Balfour, W.J.
LAUNILA, O., *see* Jonsson, J.
LAUNILA, O., ROYEN, P., and ZACKRISSON, M.: Rotation analysis of the $D^2\Sigma^+$-$X^2\Sigma$ and $E^2\Sigma$-$X^2\Sigma$ band systems of BaCl, **78**, 763
LAVOREL, B., OKSENGORN, B., FABRE, D., SAINT-LOUP, R., and BERGER, H.: Stimulated Raman spectroscopy of the *Q* branch of nitrogen at high pressure: Collisional narrowing and shifting in the 150-6800 bar range at room temperature, **75**, 397
LAW, D.W., *see* Baggott, J.E.
LAW, M.M., and DUNCAN, J.L.: C-H and C-D interbond coupling and Fermi resonance interactions in CHD_2Cl, **74**, 861
LAWLEY, K.P., AUSTIN, D., TELLINGHUISEN, J., and DONOVAN, R.J.: Oscillatory continuum fluorescence from high vibrational levels of the $E(0^+)$ ion-pair state of IBr, **62**, 1195
LAWLEY, K., JEWSBURY, P., RIDLEY, T., LANGRIDGE-SMITH, P., and DONOVAN, R.: Einstein *A*-coefficients and transition dipole moments for some ion-pair to valence transitions in I_2, **75**, 811
LAWLEY, K.P., *see* Kvaran, A.
LAZZERETTI, P., *see* Fowler, P.W.
LAZZERETTI, P., *see* Raynes, W.T.
LAZZERETTI, P., ZANASI, R., SADLEJ, A.J., and RAYNES, W.T.: Magnetizability and carbon-13 shielding surfaces for the methane molecule, **62**, 605
LAZZERETTI, P., ZANASI, R., and RAYNES, W.T.: Carbon-proton and proton-proton spin-spin coupling surfaces for the methane molecules, **66**, 831
LEBEDEV, YA, S., *see* Bresgunov, A. Yu.
LE BOITEUX S., *see* Bervas, H.
LECHUGA-FOSSAT, L. FLAUD, J.-M., CAMY-PEYRET, C., ARCAS, P., and CUISENIER, M.: The H_2S spectrum in the 1.6μm spectral region, **61**, 23
LECHNER, R.E., *see* Steiner, Th.

LE DUFF, Y., OUILLON, R., CHANDRASEKHARAN, V., and SILVI, B.: Low temperature Raman spectrum of xenon diatoms, **62**, 1065
LEE, E.M., *see* Penfold, J.
LEE, E.P.F. and DYKE, J.M.: An *ab initio* molecular orbital study of protonated water clusters, $H(H_2O)_n^+$ n = 1 to 5, at the SCF and MP2 levels, **73**, 375
LEE E.P.F., and DYKE, J.M.: An *ab initio* molecular orbital study of the anions $O_2^-.H_2O$ and $O_2^-.CO_2$, **74**, 333
LEE, E.P.F., DYKE, J.M., WILDERS, A.E., and WATTS, P.: *Ab initio* calculation of relative ion concentrations of protonated water clusters at equilibrium, **71**, 207
LEE, E.P.F.: Investigation of the C_s structure of CO_4 using *ab initio* calculations, **79**, 875
LEE E.P.F., WRIGHT, T.G., and DYKE, J.M.: Calculated dissociation energies of the alkali metal monoxides, NaO and KO. Basis set superposition error and symmetry lowering, **77**, 501
LEE, E.P.F., *see* Wright, T.G.
LEE, J., *see* Zhu, S.-B.
LEE, R.J., and CHAO, K.C.: Coordination number and thermodynamics of square-well fluid mixtures, **61**, 1431
LEE, R.J., and CHAO, K.C.: Equation of state for square-well fluids, **65**, 1253
LEE, S.A., *see* Yenice, K.M.
LEE, S.H., CUMMINGS, P.T., and STELL, G.: Statistical mechanical models of chemical reactions. IV. Solvent effects near the critical point, **62**, 65
LEFEVRE, G., *see* Broquier, M.
LEFEBVRE, R., and CHILD, M.S.: Semi-classical analysis of the stabilization method applied to tunnelling and curve crossing, **66**, 1215
LE FLOCH, A.: Revised molecular constants for the ground state of CO, **72**, 133
LE FLOCH, A., ROSTAS, J., and SCHAMPS, J.: The $A^1\Pi \sim D^1\Delta$ rotation-electronic interaction in CO, **63**, 677
LEFORESTIER, C., and MILLIE, P.: Theoretical study of the IR excitation of the ClNO molecule in a multimode laser field, **65**, 33
LEGGETTER, S., and TILDESLEY, D.J.: The computer simulation of adsorbed hydrocarbons, **68**, 519
LEHMANN, K.K.: Beyond the x -*K* relations. Calculations of 1-1 and 2-2 resonance constants with application to HCN and DCN, **66**, 1129
LEICKNAM, J.-CL., *see* Bouachir, M.
LEITNER, A.: Second-harmonic generation in metal island films consisting of oriented silver particles of low symmetry, **70**, 197
LEITNER, A., *see* Kümmerlen,J.
LEONE, S.R., *see* Meyer, H.
LOY, R.J., *see* Slee, T.
LESLIE, M., *see* Michopoulos, Y.
LE SUEUR, C.R., *see* McDowell, S.A.
LE SUEUR, C.R., MILLER, S., TENNYSON, J., and SUTCLIFFE, B.T.: On the use of variational wavefunctions in calculating vibrational band intensities, **76**, 1147
LE SUEUR, C.R., and STONE, A.J.: Practical schemes for distributed polarizabilities, **78**, 1267
LESZCZYNSKI, J., *see* Kwiatkowski, J.S.
LETELIER, J.R., *see* Acevedo, R.
LEVANT, D., *see* Moreh, R.
LEVELT SENGERS, J.M.H., and GIVEN, J.A.: Critical behaviour of ionic fluids, **80**, 899
LEVESQUE, D., *see* Caillol, J.M.
LEVESQUE, D., and VERLET: Molecular dynamics calculations of transport coefficients, **61**, 143
LEVESQUE, D., *see* Vermesse, J.
LEVESQUE, D., *see* Weis, J.J.
LEVESQUE, D., *see* Zarragoicoechea, G.J.
LEVINE, R.D., *see* Muga, J.G.
LEVINE, Y.K.: Monte Carlo dynamics study of *cis* and *trans* unsaturated hydrocarbon chains, **78**, 619
LI, K.Y., ZIMMERMAN, D.S., and BURNELL, E.E.: Orientational order of planar solutes in a zero average electric field gradient nematic environment, **78**, 673
LI LI, QINGSHI ZHU and FIELD, R.W.: The hyperfine structure of the Na_2 4 $^3\Sigma_g^+$ state, **66**, 685

LI, M., *see* Coxon, J.A.
LI, S., *see* Eggen, B.R.
LI, X., and ZHANG, Q.: A note on permutation symmetry in many-particle systems, **67**, 525
LI, Y., CARTER, S., HIRSCH, G., and BUENKER, R.J.: Theoretical calculation of the potential surfaces and vibrational frequencies of the $A^2\Sigma^+$ and $X^2\Pi$ electronic states of the NCO radical, **80**, 145
LI, Z.X., LU, J.R., STYRKAS, D.A., THOMAS, R.K., RENNIE, A.R., and PENFOLD, J.: The structure of the surface of ethanol/water mixtures, **80**, 925
LI, Z., and FRANCISCO, J.S.: Laser-induced flurescence spectroscopy of the trifluoroacetyl radical CF_3CO, **79**, 1127
LIN, S.H., *see* Alden, R.G.
LINDBERG, P., RAYBONE, D., SALTHOUSE, J.A., WATKINSON, T.M., and WHITEHEAD, J.C.: The production of electronically-excited species from the photolysis of N_2H_4 and N_2D_4 at 193 nm, **62**, 1297
LINDER, B., *see* Kromhout, R.A.
LINDER, B., and KROMHOUT, R.A.: Effect of van der Waals interaction on Raman transitions. II. **67**, 1181
LINDER, R., *see* Strand, D.
LINDNER, U., *see* Knöckel, H,.
LINGHAM, K.V., *see* Ravi Kumar, R.
LINSE, P., and HALLE, B.: Counterion N.M.R. in heterogeneous aqueous systems. A molecular dynamics simulation study of the electric field gradient, **67**, 537
LINSE, P., *see* Härtl, W.
LIPPENS, G., *see* Prevost, M.
LIPPENS, G., *see* Van Bell, D.
LIPPENS, G., VAN BELLE, D., WODAK, S.J., and JEENER, J.: T_1 relaxation time of water from a molecular dynamics simulation, **80**, 1469
LIPPMAA, E., *see* Samoson, A.
LIPSON, R.H., *see* Dabrowski, I.
LIPSON, R.H.: Spectra of rare gas hydrides. III. $^2\Pi$-$^2\Sigma$ transitions of argon hydride, **65**, 1217
LIPSON, R.H., and HOY, A.R.: A vacuum ultaviolet laser study of IBr, **68**, 1311
LIPUS, K., BACHEM, E., and URBAN, W.: Vibration-rotation spectroscopy of the CrH radical in its $X^2\Sigma^+$ ground state by CO-Faraday laser magnetic resonance, **73**, 1041
LIPUS, K., BACHEM, E., and URBAN, W.: Direct observation of fine structure transitions within the $X^2\Delta$ ground state of the NiH radical by CO_2-Faraday laser magnetic resonance, **75**, 945
LIPUS, K., NELIS, TH., BACHEM, E., and URBAN, W.: Vibration rotation spectroscopy of the CoH radical in its $X^3\Phi_4$ ground state by Co-Faraday laser magnetic resonance, **68**, 1171
LIPUS, K., SIMON, U., BACHEM, E., NELIS, TH., and URBAN, W.: Direct observation of the fundamental vibration-rotation transitions within the NiD $X^2\Delta_{5/2}$ ground state by CO-Faraday-L.M.R. spectroscopy and zero field transitions in NiH, **67**, 1431
LIPUS, K., *see* Stackmann, V.
LIPUS, K., *see* Towle, J.P.
LIPUS, K., URBAN, W., EVENSON, K.M., and BROWN, J.M.: Laser magnetic resonance spectroscopy of the NiD radical in the far- and mid-infrared, **79**, 571
LIRA, L., *see* del Rio, F.
LISCHKA, H., *see* Kofranek, M.
LISTERUD, J., and DROBNY, G.: Symmetry and isotropic coherence transfer. I. Computations for two-spin systems, **67**, 97
LISTERUD, J., GLASER, S.J., and DROBNY, G.P.: Symmetry and isotropic coherence transfer. II. Multi spin calculations using a Young tableaux formulation, **78**, 629
LIU, W.-K., and DICKINSON, A.S.: Classical limits of generalized cross-sections for atom- molecule systems, **70**, 253
LIU, W.-K., and DICKINSON, A.L.: Multipole cross-sections in polarized laser fluorescence for atom-diatom systems, **71**, 1117
LIU, W.-K., DICKINSON, A.S., and MCCOURT, F.R.W.: Comparison of quantum and classical calculations of thermal-conductivity cross-sections governing the Senftleben-Beenakker effect for HD-He mixtures, **71**, 1131

LIU, W.-K., *see* Dickinson, A.S.
LIU, W.-K., MCCOURT, F.R.W., and DICKINSON, A.S.: Quantum and classical mechanical calculations of transport-relaxation cross sections for the HD-He interaction, **66**, 565
LIU, X., FOSTER, S.C., WILLIAMSON, J.M., YU, L., and MILLER, T.A.: The spin-rotation interactions in the methoxy radical, **69**, 357
LIU, X., and MILLER, T.A.: A symmetry-based approach to the effective Hamiltonian for symmetric top molecules in degenerate vibronic states, **75**, 1237
LIVERI, V.T., *see* Majolino, D.
LOBO, L.Q., and FONSECA, I.M.A.: Ternary contribution to the excess Gibbs energy for a liquid mixture involving molecularly simple polar components, **80**, 789
LOCKHART, G., *see* Carlile, C.J.
LODYGA, W., *see* Markarewicz, J.
LOISEL, J., *see* Dayan, E.
LOMBA, E.: An efficient procedure for solving the reference hypernetted chain equations (RHNC) for simple fluids. Illustrative results with application to phase coexistence for a Lennard-Jones fluid, **68**, 87
LOMBA, E., *see* Høye, J.S.
LOMBA, E., LOMBARDERO, M., and ABASCAL, J.L.F.: New aspects in the simulation and behaviour of polar molecular fluids, **68**, 1067
LOMBA, E., MARTIN, C., and LOMBARDERO, M.: The dipolar hard sphere fluid, Hypernetted chain approximation revisited, **77**, 1005
LOMBARDERO, M., *see* Lomba, E.
LONGERI, M., *see* Celebre, G.
LONGERI, M., *see* Chidichimo, G.
LONGERI, M., *see* Emsley, J.W.
LONNGI, P.A., *see* De Lonngi, D.A.
LOOSE, G., *see* Atamny, F.
LOPATKO, O. YA., *see* Ovsiannikov, V.D.
LOPEZ, J.M., *see* Cordero, N.A.
LOPEZ, J.M., *see* March, N.H.
LÓPEZ RODRÍGUEZ, A., and FREIRE, J.J.: Application of the rotational isomeric model to the calculation of binary interactions between flexible chains. I. Second virial coefficients of n-alkanes, **63**, 591
LÓPEZ RODRÍGUEZ, A., *see* Freire, J.J.
LÓPEZ RODRÍGUEZ, A., VEGA, C., FREIRE, J.J., and LAGO, S: Potential parameters of methyl and methylene obtained from second virial coefficients of n-alkanes, **73**, 691
LÓPEZ-QUINTELA, M.A., TOJO, C., and BUJÁN-NUÑEZ, M.C.: Fractal analysis of brownian trajectories in fluids, **65**, 1195
LÓPEZ-QUINTELA, M.A., TOJO, C., and BUJÁN-NÚÑEZ, M.C.: 'Slow-down' of diffusion coefficient in finite Brownian motion, **74**, 785
LÓPEZ-QUINTELA, M.A., and BUJÁN-NÚÑEZ, M.C.: Thermodynamic and scaling behaviour in finite diffusion-limited aggregation, **77**, 857
LORQUET, J.C., *see* Desouter-Lecomte, M.
LOTFI, A., and FISCHER, J.: Chemical potentials of model and real dense fluid mixtures from perturbation theory and simulations, **66**, 199
LOTFI, A., and FISCHER, J.: Chemical potentials of model and real dense fluid mixtures from perturbation theory and simulations (erratum), **71**, 1171
LOTFI, A., VRABEC, J., and FISCHER, J.: Vapour liquid equilibria of the Lennard-Jones fluid from the *NpT* plus test particle method, **76**, 1319
LOUNILA, J., *see* Jokisaari, J.
LOUNILA, J., WASSER, R., and DIEHL, P.: Effects of anharmonic vibrations on molecular properties, **62**, 19
LO, WAI YIN, CHAN, KWONG-YU, and HENDERSON, D.: Improved Monte Carlo simulations of the structure of ion-dipole mixtures, **80**, 1021
LU, J.R., *see* Li, Z.X.
LUBIMOV, YU. A., *see* Nabokov, O.A.
LUCAS, K., *see* Shing, K.S.

LUCKAS, M., *see* Vogelsang, R.
LUCKHAUS, D., and QUACK, M.: The far infrared pure rotational spectrum and the Coriolis coupling between υ_3 and υ_8 in $CH^{35}ClF_2$, **68**, 745
LUCKHAUS, D., *see* Ross, A.J.
LUCKHURST, G.R., *see* Adams, D.J.
LUCKHURST, G.R., *see* Counsell, C.J.R.
LUCKHURST, G.R., *see* Date, R.W.
LUCKHURST, G.R., *see* Emerson, A.P.J.
LUCKHURST, G.R., *see* Emsley, J.W.
LUCKHURST, G.R., *see* Ferrarini, A.
LUCKHURST, G.R., *see* Hamley, I.W.
LUCKHURST, G.R., *see* Heaton, N.J.
LUCKHURST, G.R., and SIMMONDS, P.S.J.: Computer simulation studies of anisotropic systems. XXI. Parametrization of the Gay-Berne potential for model mesogens, **80**, 233
LÜDEMANN, H.-D., *see* Speedy, R.J.
LUHMER, M., DEJAEGERE, A., and REISSE, J.: A comparison between the PISA model and the RAM theory; their abilities to reproduce internal energy as calculated by Monte Carlo simulations, **71**, 843
LUKS, K.D., *see* Jangkamolkulchai, A.
LUKS, K.D., *see* Green, K.A.
LUPKOWSKI, M., *see* McGuigan, D.B.
LUPKOWSKI, M., and MONSON, P.A.: Structure and thermodynamics of polar interaction site fluids, **63**, 875
LUPKOWSKI, M., and MONSON, P.A.: Phase diagrams of interaction site fluids. II. Dipolar diatomics, **67**, 53
LUSTIG, R., *see* Bohn, M.
LUSTIG, R.: Angle-average for the powers of the distance between two separated vectors, **65**, 175
LUSTIG, R., and STEELE, W.A.: On the thermodynamics of liquid propane. A molecular dynamics study, **65**, 475
LUSTIG, R., *see* Toro-Labbé, A.
LUTOVINOV, V.S., *see* Chechetkin, V.R.
LUZAR, M., THAYER, A.M., and PINES, A.: Zero field N.M.R. of uniaxial and biaxial smectic liquid crystals, **62**, 573
LYNDEN-BELL, R.M.: The orientational order/disorder phase transition of urea-paraffin inclusion compounds, **79**, 313
LYNDEN-BELL, R.M., *see* Evans, D.J.
LYNDEN-BELL, R.M., *see* Guldbrand, L.E.
LYNDEN-BELL, R.M., VAN DUIJNEVELDT, J.S., and FRENKEL, D.: Free energy changes on freezing and melting ductile metals, **80**, 801
LYNDEN-BELL, R.M., and WESTLUND, P.-O.: The effects of pressure and temperature on vibrational dephasing in a simulation of liquid CH_3CN, **61**, 1541
LYNDEN-BELL, R.M., *see* Xu, H.

MCCAFFERY, A.J., *see* Kenyon, A.J.
MCCORMICK, A.V., and CHMELKA, B.F.: Xenon adsorption in NaA zeolite cavities, **73**, 603
MCCORMICK, A,V. *see* Van Tassel, P.R.
MCCOURT, F.R.W., *see* Aziz, R.A.
MCCOURT, F.R.W., *see* Bissonnette, E.C.
MCCOURT, F.R.W., *see* Corey, G.
MCCOURT, F.R.W., *see* Hanson, E.E.
MCCOURT, F.R.W., *see* Liu, W.-K.
MCCOURT, F.R.W., *see* Maitland, G.C.
MCCOURT, F.R.W., VAN DUIJNEVELDT, F.B., VAN DAM, T., and FUCHS, R.R.: New anisotropic potential energy surfaces for N_2-Ne and N_2-Ar. The use of Hartree-Fock SCF calculations and anisotropic long-range dispersion coefficients, **61**, 109

McCOURT, F.R.W., VAN DUIJNEVELDT, F.B., VAN DAM, T., and FUCHS, R.R.: New anisotropic potential energy surfaces for N_2-Ne and N_2-Ar. The use of Hartree-Fock SCF calculations and anisotropic long-range dispersion coefficients (erratum), **65**, 757

McCOURT, F.R.W., VESOVIC, V., WAKEHAM, W.A., DICKINSON, A.S., and MUSTAFA, M.: Quantum mechanical calculations of effective collision cross-sections for He-N_2 interaction. Part 1. Viscomagnetic effect. **72**, 1347

McCOURT, F.R.W., *see* Wing-Ki Liu

McCOURT, F.R.W., *see* Wong, C.C.K.

McCOY, A.B., and SIBERT, E.L., III.: An algebraic approach to calculating rotation-vibration spectra of polyatomic molecules, **77**, 697

McDONALD, I.R., *see* Alavai, A.

McDONALD, I.R., *see* Barrat, J.-L.

McDONALD, I.R., *see* Brode, S.

McDONALD, I.R., *see* Ferrario, M.

McDONALD, I.R., *see* Forester, T.R.

McDONALD, I.R., *see* Hammonds, K.D.

McDONALD, I.R., *see* Ryckaert, K.P.

McDONALD, I.R., *see* Siepmann, J.I.

McDONALD, I.R., *see* Yashonath, S.

McDOWELL, C.A., *see* Nakai, T.

McDONALD, P.J., VIJAYARAGHAVAN, D., DEBENHAM, P.M., and HORSEWILL, A.J.: Pressure dependence of methyl tunnelling in solid diacetyl. An extension to the methyl thermometer model, **78**, 219

McDOWELL, J.J.W., *see* Francisco, J.S.

McDOWELL, S.A., LE SUEUR, C.R., BUCKINGHAM, A.D., and STONE, A.J.: Using monomer properties to obtain integrated intensities for vibrational transitions of van der Waals complexes, **77**, 823

McDOWELL, S.A.D., and BUCKINGHAM,, A.D.: A study of the induced dipole moments in Li^+F^- and Li^+ ...Ne, **80**, 1555

McEWAN, K.J., HARRISON, K.J., and MADDEN, P.A.: Polarisation and material dependence of degenerate four-wave mixing transients in molecular fluids, **69**, 1025

McGUIGAN, D.B., LUPKOWSKI, M., PAQUET, D.M., and MONSON, P.A.: Phase diagrams of interaction site fluids. I. Homonuclear 12-6 diatomics, **67**, 33

McGUIGAN, D.B., and MONSON, P.A.: Vapour-liquid critical lines predicted by distribution function theories, **62**, 3

McKEAN, D.C., *see* Baggott, J.E.

McKEE, M.L., *see* Ekern, S.P.

McKELLAR, A.R.W., *see* Howard B.J.

McKELLAR, A.R.W., *se* Randall, R.W.

McLAUCHLAN, K.A., *see* Batchelor, S.N.

McLAUCLHAN, K.A., *see* Hamilton, C.A.

McLAUCHLAN, K.A., and NATTRASS, S.R.: Experimental studies of the spin-correlated radical pair in micellar and microemulsion media; MARY, RYDMR B_0 and RYDMR B_1 spectra, **65**, 1483

McLAUCHLAN, K.A., and STEINER, U.E. The spin-correlated radical pair as a reaction intermediate, **73**, 241

McLAUCHLAN, K.A., *see* Valyaev, V.I.

McLAUGHLIN, E., *see* Gupta, S.

McLAUGHLIN, E., *see* Sediawan, W.B.

McLAUGHLIN, I.L., *see* Gianotti, R.D.

McLAUGHLIN, I.L. *see* Jun Wang

McMAHON, P.D.: The effects of three-body dispersion interactions on liquid-liquid phase equilibriumn, **66**, 647

McMEEKING, R.F., *see* Brown, C.A.

McMILLAN, K., COPLAN, M.A., TOSSELL, J.A., and MOORE, J.H.: Experimental orbital momentum distribution and bonding interactions. Part II. The organometallic complex (η^4-1,3, -C_4H_6)-$Fe(CO)_3$, **73**, 619

McNAB, I.R., *see* Carrington, A.
McNAUGHTON, D., *see* Brown, R.D.
McNICHOLS, A. and CARRINGTON, T., JR.: An adiabatic energy-level expression for anharmonic hydrogen-bonded systems, **71**, 1155
McQUARRIE, D.A., *see* Feller, S.E.
McQUARRIE, D.A., *see* Rowlinson, J.S.
MACHADO, F.B.C., and ORNELLAS, F.R.: A theoretical study of the BeF molecule in the $X^2\Sigma^+$ state, **67**, 1129
MACHADO, F.B.C., *see* Ornellas, F.R.
MACHIDA, K., *see* Nakamura, R.
MACHIDA, K., *see* Katō, T.
MACHO, V., *see* Dahm, J.
MACIA, E., *see* Dominguez-Adame, F.
MACLEAN, C., *see* Bastiaan, E.W.
MACLEAN, C., *see* Huis, L.
MACPHERSON, A.K., *see* Vladimiroff, T.
MACPHERSON, P.A., *see* Vladimiroff, T.
MADDEN, P.A., *see* Evans, G.T.
MADDEN, P.A., *se* Eldridge M.D.
MADDEN, P.A., *see* McEwan, K.J.
MADDEN, P.A, *see* Remler, D.K.
MADDOX, M.W., *see* Baram, A.
MADER, G.M., *see* Jäger, W.
MADER, H., *see* Nicolaisen, H.-W.
MADER, H., *see* Wolf, P.
MADI, Z.L., *see* Schulte-Herbreggen, T.
MADURA, J.D., PETTITT, B.M., and CALEF, D.F.: Water under high pressure, **64**, 325
MAESO, M., SOLANA, J.R., and AMOROS, J.: More accurate equations of state for non-spherical hard-particle fluids, **76**, 1269
MAESO, M.J., and SOLANA, J.R.: An accurate equation of state for hard Gaussian overlap fluids from a generalized Carnahan-Starling method, **79**, 449
MAESO, M.J., and SOLANA, J.R.: Equation of state for hard ellipsoid-of-revolution fluids from a direct summation of the virial series, **79**, 1365
MAGAZU, S., *see* Maisano, G.
MAGAZU, S., *see* Majolino, D.
MAGAZU, S., MAJOLINO, D., MALLAMACE, F., MIGLIARDO, P., ALIOTTA, F., VASI, C., D'APRANO, A., and DONATO, D.I.: Velocity and damping of thermal phonons in isomeric alcohols, **66**, 819
MAGER, T., BERTAGNOLLI, H., DEGENHARDT, D., and FRAHM, R.: The liquid-phase structure of the tetrabromomethane-toluene complex. A differential anomalous X-ray scattering study, **73**, 587
MAGHEZZI, S., *see* Labani, B.
MAGILL, J.H., *see* Zemke, K.
MAGNASCO, V., and FIGARI, G.: One-centre calculation of dispersion coefficients between ground state H atoms from pseudostate decomposition of static multipole polarizabilities, **62**, 1419
MAGNASCO, V., and FIGARI, G.: A generalized multipole expansion for molecular interactions, **67**, 1261
MAGNASCO, V., FIGARI, G., and COSTA, C.: Perturbation calculations of nonexpanded interactions in small atomic and molecular systems, **75**, 1133
MAGNUSSON, K.O., WIKLUND, S., DUDDE, R., and REIHL, B.: Interface formation of alkali metals on Si(111) surfaces, **76**, 909
MAHDI, W., *see* Atamny, F.
MAHMOOD, M.F.: Collisional studies involving metastable species ($N_2(A)$ and $HgBr_2/CH_3$ collisions), **68**, 959
MAIER, J.P., *see* Celii, F.G.
MAIER, J.P., *see* Hanratty, M.A.
MAIER, J.P., *see* King, M.A.

MAIER, J.P., *see* Rosslein, N.
MAÏNOS, C.: Molecular axis orientation and transitional path effects in the rotational structure of multiphoton transitions, **73**, 1241
MAINOS, C., and CASTEX, M.C.: The single path rotational structure of *n*-photon transitions in diatomic molecules, **68**, 615
MAISANO, G., MAJOLINO, D., MIGLIARDO P., VENUTO, S. ALIOTTA, F., MAGAZU, S., and VASI, C.: Hyperacoustic properties and local structure in hydrated molton salts, **72**, 547
MAISANO, G., MAJOLINO, D., MIGIARDO, P., VENUTO S., ALIOTTA, F., and MAGAZU, S.: Sound velocity and hydration phenomena in aqueous polymeric solutions, **78**, 421
MAITI, A.K., *see* Rodrigues, S.V.
MAITLAND, G.C., *see* Corey, G.C.
MAITLAND, G.C., MUSTAFA, M., WAKEHAM, W.A., and MCCOURT, F.R.W.: An essentially exact evaluation of transport cross-sections for a model of the helium-nitrogen interaction, **61**, 359
MAITLAND, G.C., MUSTAFA, M., and WAKEHAM, W.A.: Close-coupled calculations of transport cross-sections for a highly quantal system, **62**, 397
MAJER, W., *see* Hettner, W.
MAJIMA, T., *see* Matsumoto, Y.
MAJOLINO, D., *see* Magazú, S.
MAJOLINO, D., *see* Maisano, G.
MAJOLINO, , D., MIGLIARDO, P., ALIOTTA, F., MAGAZU, S., VASI, C., D'APRANO, A., DONATO, D.I., and LIVERI, V.T.: Relaxation phenomena in mixed isomeric alcohols by Mandelstam-Brillouin scattering, **73**, 27
MAKAREWICZ, J.: Hartree theory for rovibrational states of molecules, **61**, 547
MAKAREWICZ, J.: Reduced density matrices and reduced local operators for a rotating-vibrating molecule, **66**, 113
MAKAREWICZ, J.: Semiclassical and quantum mechanical pictures of the ro-vibrational motion of triatomic molecules, **69**, 903
MAKAREWICZ, J., and LODYGA, W.: Self-consistent internal axes for a rotating-vibrating triatomic molecule, **64**, 899
MAKAREWICZ, J., and PYKA, J.: Centrifugal stabilization and destabilization of molecular geometry and clustering of rovibrational energy levels in the H_2O, **68**, 107
MAKINEN, M.W., *see* Wells, G.B.
MAKOVSKY, N.N., Structure of the surfactant-water interface, **72**, 235
MAKOVSKY, N.N., *see* Antonchenko, V. Ya.
MALBRUNOT, P., *see* Vidal, D.
MALDIVI, P., *see* Carpentier, L.
MALDIVI, P., *see* Giroud-Godquin, A.M.
MALESCIO, G.: Excess electrons in molten salts. Polaron theory of dilute Cs-CsI solutions, **69**, 895
MALHOTRA, R., *see* Harris, K.R.
MALIJEVSKY, A., *see* Labik, S.
MALIJEVSKY, A., LABIK, S., and SMITH, W.R.: Prediction of the amorphous structure of the hard sphere system up to random close packing, **72**, 193
MALIJEVSKY, A., POSPISIL, R., and LABIK, S.: Calculation of thermodynamic quantities of inert-gas fluids by means of the *RHNC* and modern pair potentials, **61**, 533
MALIJEVSKY, A., *see* Pospisil, R.
MALIJEVSKY, A., POSPISIL, R., SMITH, W.R. and LABIK, S.: The Ornstein-Zernike equation for hard spheres near a hard wall. A rapid method of numerical solution and an accurate new RHNC theory, **72**, 199
MALIJEVSKY, A., POSPISIL, R., SMITH, W.R. and LABIK, S.: The Ornstein-Zernike equation for hard spheres near a hard wall. A rapid method of numerical solution and an accurate new RHNC theory (Erratum), **75**, 981
MALINIAK, A., and LAAKSONEN, A.: Molecular dynamics computer simulation study of the solvation of quinuclidine in benzene, **62**, 489
MALLAMACE, F., *see* Magazü, S.
MALLORY, F.B., *see* Beckmann, P.A.
MAN, P.P.: Measurement of quadrupolar coupling with a two-pulse sequence in solid-state N.M.R., **69**, 337

MAN, P.P.: Study of a spin-3/2 system by a spin-echo sequence, **72**, 321
MAN, P.P.: Double-quantum coherence detection in a spin-3/2 system excited by two consecutive pulses, **76**, 1119
MAN, P.P.: Analytical expression for the spin-5/2 line intensities, **78**, 307
MANESCALCHI, F., *see* Caminati, W.
MANIERO, A.L., *see* Brustolon, M.
MANIERO, A.L., *see* Caciuffo, R.
MANIERO, A.L. BRUSTOLON, M., OTTAVIANO, M.F., RIZZOLI, C., SCARABOTTO, P., UGOZZOLI, F., CARLONI, P., and GRECI, I.: EPR and ENDOR study on mixed crystals of an indolinone nitroxide radical and the isoelectronic ketone. I. X-ray structure of pure components and ENDOR of isolated radicals in mixed crystals, **73**, 1
MANIERO, A.L. BRUSTOLON, M., OTTAVIANO, M.F., RIZZOLI, C., SCARABOTTO, P., UGOZZOLI, F., CARLONI, P., and GRECI, I.: EPR and ENDOR study on mixed crystals of an indolinone nitroxide radical and the isoelectronic ketone. II. EPR and ENDOR investigation on radical pairs in mixed crystals, **73**, 15
MANOHARAN, P.T., *see* Sreehari, N.
MANN, M.E., MARSHALL, C.H., and HAYMET, A.D.J.: Nematic liquid crystals. A Monte Carlo simulation study in higher dimensions, **66**, 493
MANSOUR, K.A., MURAD, S., and POWLES, J.G.: A computer simulation study for model liquid ammonia-time correlation functions, **65**, 785
MANYROV, I.R., *see* Gaisin, N.K.
MANZ, J., *see* Karrlein, W.
MARCH, N.H., ALONSO, J.A., and LOPEZ, J.M.: Potential energy curve of H_2 related to mirror-plane ground-state electron density, **79**, 1143
MARCH, N.H., *see* Cordero, N.A.
MARCH, N.H., *see* Golden, K.I.
MARCH, N.H., and WIND, P.: An asymptotic spatial generalization of Kato's theorem for really heavy atoms in nonrelativistic theory, **76**, 1119
MARCH, N.H., and WIND, P.: Origin of the linear dependence with atomic number of correlation energies in neutral atoms, **77**, 791
MARCHI, M., *see* Kurtović, Z.
MARCHON, J.C., *see* Carpentier, L.
MARCHON, J.C., *see* Giroud-Godquin, A.M.
MARCONI, U.M.B., and VAN SWOL, F.: Structure effects and phase equilibria of Lennard-Jones mixtures in a cylindrical pore. A non-local density-functional theory, **72**, 1081
MARECHAL, G., RYCKHAERT, J-P., and BELLEMANS, A.: The shear viscosity of a *n*-butane by equilibrium and non-equilibrium molecular dynamics, **61**, 33
MARESCH, G.G., *see* Dahm, J.
MARIAN, C.M., *see* de Vivie, R.
MARIAN, C.M., *see* Matsushita, T.
MARIANI, L., *see* Giorgina, M.G.
MARKS, A.J., MURRELL, J.N., STACE, A.J., and BUSCHER, H.: A model for the computer simulation of chemical reactions in the condensed phase, **65**, 1153
MAROULIS, G.: SDTQ-MPPT(4) electric moments and static polarizabilities for $Li_2(X^1\Sigma_g^+)$, **63**, 299
MAROULIS, G.: On the dipole polarizability of HCl, **74**, 131
MAROULIS, G.: Dipole moment and polarizability of hydrogn selenide, **76**, 1303
MAROULIS, G.: Accurate dipole polarizability for $Cl_2(X^1\Sigma_g^+)$, **77**, 1085
MAROULIS, G., and THAKKAR, A.J.: *Ab initio* static polarizabilities and multipole moments of I_2, **73**, 1235
MARSAULT, J.P., *see* Bizot, P.
MARSAULT-HERAIL, F., *see* Bizot, P.
MARSHALL, C.H., *see* Mann, M.E.
MARTI, J., ANDRÉS, J.L., BERTRÁN, J., and DURAN, M.: Molecular electric properties and nuclear and vibrational relaxation. An *ab initio* study of HF, CH_4 and C_2H_4, **80**, 625
MARTINEZ-HEYA, B., *see* Ferrero, F.S.
MARTÍNEZ, J.L., *see* Chahid, A.

MARTINEZ, J.L., *see* Criado, A.
MARTINEZ, M.T., *see* Brouard, M.
MARTEAU, PH., *see* Guillot, B.
MARTIN, C., *see* Lomba, E.
MARTIN, J.P.D., *see* Bowden, G.J.
MARTIN, N.A., *see* Burie, J-R.
MARTIN, P.A., *see* Davies, P.B.
MARTINEZ, M.T., *see* Brouard, M.
MARTINEZ-CASAS, S.E., *see* Alejandre, J.
MARUANI, J., *see* Mezey, P.G.
MARUO, T., RATAJCZAK, R.D., and JONES, M.T.: An ESR study of ion pairing in solutions of the alkali metal salts of tetracyanoquinodimethan (TCNQ) and tetrafluorotetracyanoquinodimethan (TCNQF), **73**, 1365
MASELLI, P., *see* Buontempo, U.
MASLEN, I., *see* Jayatilaka, D.
MASON, E.A., *see* Ihm, G.
MASON, E.A., *see* Iinuma, K.
MASON, E.A., SIREGAR, J.J., and HUANG, Y.: Simplified calculation of quantum corrections to the virial coefficients of hard convex bodies, **73**, 1171
MASON, S.M., and TUCKETT, R.P.: Computer simulation of the rotational structure of vibronic bands of CF_4^+ and SiF_4^+ D^2A_1-C^2T_2, **62**, 175
MASON, S.M., and TUCKETT, R.P.: The D^2A_1-C^2T_2 emission band system of GeF_4^+, **62**, 979
MASTERS, A.J., *see* Allen, M.P.
MASTERS, A.J., *see* Treloar, R.L.
MASTERS, A.J., *see* Whittle, M.
MATIAS, M.A., and VARANDAS, A.J.C.: Atom-molecule dispersion-energy coefficients and their dependence on the intramolecular coordinate: A-H_2 systems, **70**, 623
MATSUMOTO, M., OHTORI, N., OKAZAKI, S., and OKADA, I.: Raman spectroscopic study of vibrational and rotational relaxation of the NO_3^- ion in molten binary systems (Li-K)NO_3 and (Na-K)BI_3, **68**, 671
MATSUMOTO, M., *see* Okazaki, S.
MATSUMOTO, Y., MAJIMA, T., and TAKAMI, M.: Free jet infrared absorption spectroscopy of the CO stretching υ_6 fundamental of $Fe(CO)_5$, **61**, 1045
MATSUMOTO, Y., *see* Takami, M.
MATSUSHITA, T., KLOTZ, R., MARIAN, C.M., and PEYERIMHOFF, S.D.: *Ab initio* calculations of the radiative lifetime of the $a^1\Delta$ and $b^1\Sigma^+$ states in SeO molecule, **62**, 1385
MATSUZAWA, H., *see* Kobayashi, H.
MATTHEWS, G.P., *see* Hunter, I.N.
MATYUSHOV, D.V.: A molecular theory of electron transfer reactions in polar liquids, **79**, 795
MAULWURF, M., *see* Stetter, M.
MAUSS, Y., *see* Grucker, D.
MAVERICK, E., and DUNITZ, J.D.: Rotation barriers in crystals from atomic displacement parameters, **62**, 451
MAVROYANNIS, C.: Dynamic effects of surface plasmons on the lifetimes of neutral excited rare-gas atoms physisorbed on metal surfaces. Radiative and nonradiative processes, **64**, 457
MAVROYANNIS, C.: Dynamics effects of surface plasmons on the lifetimes of neutral excited rare-gas atoms physisorbed on metal surfaces. II. Numerical results, **65**, 977
MAY, P.S., REIDD, M.F., and RICHARDSON, F.S.: Optical spectra, energy levels and crystal-field analysis of Sm^{3+} in Na_3 [$(Sm(oxydiacetate)_3] \cdot 2NaClO_4 \cdot 6H_2O$, **61**, 1455
MAY, P.S., REIDD, M.F., and RICHARDSON, F.S.: Electric dipole intensity parameters for the samarium $4f \rightarrow 4f$ transitions in $Na_3[Sm(oxydiacetate)_3] \cdot 2NaClO_4 \cdot 6H_2O$, **61**, 1471
MAY, P.S., REID, M.F., and RICHARDSON, F.S.: Circular dichroism spectra and electronic rotatory strengths of the samarium $4f \rightarrow 4f$ transitions in $Na_3[Sm(oxydiacetate)_3] \cdot 2BaClO_4 \cdot 6H_2O$, **62**, 341
MAYER, K., *see* Hettner, W.
MAYERS, J., *see* Andreani, C.
MAZZACURATI, V., *see* Benassi, P.

MAZZACURATI, V., *see* De Santis, A.
MAZZACURATI, V., *see* Gallo, P.
MAZZACURATI, V., and RUOCCO, G.: Evaluation of Brillouin scattering intensities from rare gas crystals. I. A pure dipole induced dipole theory, **61**, 1391
MAZZACURATIO, V., and RUOCCO, G.: On the self-consistent equation for the microscopic local electric field in dielectric systems, **73**, 745
MEATH, W.J., *see* Aziz, R.A.
MEATH, W.J., *see* Dham, A.K.
MEATH, W.J., *see* Kondo, A.E.
MEATH, W.J., *see* Kumar, A.
MEATH, W.J., *see* Sachiko Nakai
MEATH, W.J., *see* Watanabe, K.
MEATH, W.J., *see* Wheatley, R.J.
MECKL, S., and ZEIDLER, M.D.: Self-diffusion measurements of ethanol and propanol, **63**, 85
MEDEROS, L., *see* Tjipto-Margo, B.
MEDVEDEV, N.N., *see* Naberukhin, Y.I.
MEENAKSHI, A., INNES, K.K., and BICKEL, G.A.: The 1900 Å band system of HCN and its isotopes. One or two excited states? **68**, 1179
MEERTS, J., *see* de Haag, P.U.
MEHLIG, B., HEERMANN, D.W., and FORREST, B.M.: Exact Langevin algorithms, **76**, 1347
MEHRING, M., *see* Rautter, J.
MEHRING, M., *see* Sariciftci, N.S.
MEHTA, M., and KOFKE, D.A.: Implementation of the Gibbs ensemble using a thermodynamic model for one of the coexisting phases, **79**, 39
MEIJERS, S.M., *see* Wang, D.M.
MELANDRI, S., *see* Caminati, W.
MELCHIONNA, S., CICCOTTI, G., and HOLIAN, B.L.: Hoover *NPT* dynamics for systems varying in shape and size, **78**, 533
MELLINON, P., *see* Broyer, M.
MELONE, S., *see* Caciuffo, R.
MELROSE, J.R.: Brownian dynamics simulation of dipole suspensions under shear: the phase diagram, **76**, 635
MELROSE, J.R., *see* Heyes, D.M.
MELROSE, J.R., and SINGER, K.: An investigation of supercooled Lennard-Jones argon by quantum mechanical and classical Monte Carlo simulation, **66**, 1203
MÉNDEZ, B., *see* Dominguez-Adame, F.
MENZEL, R.: Modelling excited states absorption (ESA) measurements including the photo-physical hole burning effect with rate equations, **68**, 161
MERCER, J.M.: Effective isotropic dipole-dipole pair potential, **69**, 625
MERCHAN, M., *see* Garcia-Cuesta, I.
MERCHÁN, M., *see* González-Luque, R.
MERKT, F., and SOFTLEY, T.P.: Prediction of rotational line intensities in doubly-enhanced four-wave mixing (DEFMI) spectroscopy, **72**, 787
MERLO, V., *see* Andreani, C.
MERONI, A., REATTO, L., and TAU, M.: Differential approach to the theory of fluids in the presence of two- and three-body potentials and study of the critical point of krypton, **80**, 977
MESTECHKIN, M.M., and WHYMAN, G.E.: Structural influence on ferromagnetic ordering in quasi-one-dimensional systems, **69**, 775
MEYER, H., and LEONE, S.R.: Steady state model for the collision induced rotational alignment of molecular ions in electric drift fields, **63**, 705
MEYER, R., *see* Caminati, W.
MEZEI, M.: Grand-canonical ensemble Monte Carlo study of dense liquid. Lennard-Jones soft spheres and water, **61**, 565
MEZEI, M.: Test of the overlap ratio method on the calculation of the aqueous hydration free energy difference between acetone and dimethylamine, **65**, 219

MEZEI, M.: Excess free energy of different water models computed by Monte Carlo methods (erratum), **67**, 1205
MEZEI, M.: Grand-canonical ensemble Monte Carlo study of dense liquid. Lennard-Jones, soft spheres and water (erratum), **67**, 1207
MEZEY, P.G., and MARUANI, J.: The concept of 'syntopy'. A continuous extension of the symmetry concept for quasi-symmetric structures using fuzzy-set theory, **69**, 97
MHIN, BYUNG JIN *see* Xie, Yaoming
MICHALIK, J., *see* Van der Pol, A.
MICHELETTI, L., *see* Brustolon, M.
MICHELOT, F., and SCHWARTZMANN, T.: Symmetry of molecular properties. I. Theory and applications to vibration-rotation properties of spherical top molecules, **80**, 1269
MICHELS, J.P.J., *see* Joslin, C.G.
MICHELS, J.P.J., *see* Smit, B.
MICHOPOULOS, Y., ADAM, C.D., and LESLIE, M.: Atom-atom potentials and the crystal structure simulation of long linear chain carboxylic acids, **72**, 899
MIER-Y-TERAN, L., TANG, Z., DAVIS, H.T., SCRIVEN, L.E., and WHITE, H.S.: Non-local free-energy density-functional theory applied to the electrical double layer. Part II:2:1 electrolytes, **72**, 817
MIER-Y-TERAN, L., *see* Zixiang Tang
MIGLIARDO, P., *see* Maisano, G.
MIGLIARDO, P., *see* Magazú,S.
MIGLIARDO, P., *see* Majolino, D.
MIJOULE, C., *see* Bouteiller, Y.
MIKAMI, M., *see* Adya, A.K.
MILLAR, G.J., ROCHESTER, C.H., HOWE, C., and WAUGH, K.C.: A combined infrared, temperature programmed desorption and temperature programmed reaction spectroscopy study of CO_2 and H_2 interactions on reduced and oxidized silica-supported copper catalysts, **76**, 833
MILLER, J.B., *see* Cory, D.G.
MILLER, S., *see* Ayllon, A.G.
MILLER, S., *see* Le Sueur, C.R.
MILLER, S., TENNYSON, J., and SUTCLIFFE, B.T.: First principles calculation of rotational and ro-vibrational line strengths. Spectra for H_2D^+ and D_2H^+, **66**, 429
MILLER, T.A., *see* Hsu, Y.-C.
MILLER, T.A., *see* Liu, Xianming.
MILLFIELD, K.F., *see* Moha, M.
MILLIE, P., *see* Leforestier, C.
MILLOT, C., and RIVAIL, J.-L.: Molecular dynamics simulation of the TIPS model of 1,2-dichloroethane in the liquid phase, **77**, 157
MILLOT, C., and STONE, A.J.: Towards an accurate intermolecular potential for water, **77**, 439
MILLS, I.M.: Anharmonicity and local mode effects in the vibrational spectra of $Ni(CO)_4$ and $Co(CO)_3NO$, **61**, 711
MILLS, I.M., *see* Baggott, J.E.
MILLS, I.M., *see* Holland, J.K.
MINH THO NGUYEN, TAE-KYU HU, and YOSHIMINE, M.: the LiC_2H_2 and NaC_2H_2 adducts. Is sodium-vinylidene observed in matrix reaction of sodium with acetylene?, **77**, 921
MIRALLES-SABATER, J., *see* Garcia-Guesta, I.
MISAWA, M., *see* Ichikawa, K.
MITCHELL, C.E.J., *see* Temme, F.P.
MITEVA, M., *see* Zhelyaskov, V.
MITSUAKI GINOZA: Simple MSA solution and thermodynamic theory in hard-sphere Yukawa system, **71**, 145
MITSUDA, Y., *see* Yamada, T.
MITTAG, U., SAMIOS, J., and DORFMULLER, TH.: Molecular dynamics simulation of the liquid mixtures CCl_4/CS_2. I. Thermodynamic and structural properties, **66**, 51

MITTAG, U., SAMIOS, J., DORFMUELLER, TH., GUENSTER, ST., ZEIDLER, M.D. and CHIEUX, P.: A comparative molecular dynamic neutron scattering study of the liquid mixture carbon tetrachloride/carbon disulphide, **67**, 1141
MÖBIUS, K., *see* Jaegermann, P.
MOCHIZUKI, K., *see* Konami, H.
MOGNASCHI, E.R., and CHIERICO, A.: Association behaviour of pure polar liquids: dielectric properties of heptadecanoic and nonadecanoic acids, **68**, 241
MOGNASCHI, E.R., LABORANTI, L.M., and CHIERICO, A.: On the correlation factor of pure polar fluids whose molecules dimerize to nonpolar dimers, **74**, 211
MOHALLEM, J.R., *see* Chacham, H.
MOHALLEM, J.R., *see* da Costa, H.F.M.
MOHAN, M., MILFELD, K.F., and WYATT, R.E.: A new general *R*-matrix theory of collinear reactions and its application to the H + H_2 reaction, **70**, 1085
MOHAN, V., *see* Karrlein, W.
MOHANTY, U., *see* Singh, U.P.
MOHEBBI, A., and SHAKA, A.J.: *J*-compensated homonuclear cross polarization in NMR spectroscopy, **78**, 29
MOISEYEV, N., *see* Engdahl, E.
MOLIN, YU. N., *see* Valyaev, V.I.
MÖLLER, D., and FISCHER, J.: Vapour liquid equilibrium of a pure fluid from test particle method in combination with *NpT* molecular dynamics simulations, **69**, 463
MÖLLER, D., OPRZYNSKI, J., and FISCHER, J.: Thermodynamic properties of mixtures with linear molecules from WCA-type perturbation theory in comparison with MD results, **75**, 1455
MÖLLER, d., OPRZYNSKI, J., MÜLLER, A., and FISCHER, J.: Prediction of thermodynamic properties of fluid mixtures by molecular dynamics simulations: methane-ethane, **75**, 363
MONCRIEFF, D., *see* Wilson, S.
MONOT, P., *see* Attal-Trétout, B.
MONSON, P.A.: The properties of inhomogeneous square-well mixtures in one dimension, **70**, 401
MONSON, P.A., *see* Dubey, G.S.
MONSON, P.A., *see* Finn, J.E.
MONSON, P.A., *see* Kierlik, E.
MONSON, P.A., *see* Lupkowski, M.
MONSON, P.A., *see* McGuigan, D.B.
MONSON, P.A., *see* Paras, E.P.A.
MONTAGUE, D.G., *see* Farman, H.
MONTERO, J.C.G., *see* Powles, J.G,
MONTGOMERIE, C.A., *see* Carrington, A.
MONTGOMERIE-LEACH, C.A., *see* Carrington, A.
MONTONE, A., and SACCHETTI, F.: Structure of the amorphous phase of sodium hydroxide, **69**, 1073
MOOIJ, G.C.A.M., and FRENKEL, D.: Novel scheme to compute chemical potentials of chain molecules on a lattice, **74**, 41
MOOIJ, G.C.A.M., DE LEEUW, S.W., WILLIAMS C.P., and SMIT, B.: Free-energy computations for mixtures of Stockmayer and polarizable Lennard-Jones fluids, **71**, 909
MOORE, E.A., *see* Mortimer, M.
MOORE, J.H., *see* McMillan, K.
MORADI, M., and RICKAYZEN, G.: The structure of a hard sphere fluid mixture confined to a slit, **66**, 143
MORADI, M., and RICKAYZEN, G.: An approximate density functional for an inhomogeneous dipolar fluid, **68**, 903
MORALDI, M., *see* Dore, P.
MORALES, J.J., and SINGER, K.: Path integral simulation of the free energy of (Lennard Jones) neon, **73**, 873
MORALES, J.J., *see* Velarde, J.M.
MORAN, G., *see* Stranger, R.
MORAWITZ, H., *see* Winkler, R.G.
MOREAU, M., *see* Simonin, J.P.

MOREH, R., and LEVANT, D.: NRPS study of nitric oxide adsorption on activated carbon fibre, **69**, 735
MOREH, R., and SHAHAL, O.: Nuclear resonance photon scattering study of nitric oxide absorbed on graphite, **65**, 279
MORGNER, H., *see* Hertzner, A.W.
MORGNER, H., OBERBRODHAGE, J., RICHTER, K., and ROTH, K.: Surface segregation of a bindary liquid mixture as studied by metastable impace electron spectroscopy, **73**, 1295
MORGNER, H., OBERBRODHAGE, J., and RICHTER, K.: The first stages of lipid layer formation. A metastable impact electron spectroscopy study of egg lecithin dissolved in hydroxy-propionitrile, **76**, 813
MORGNER, H., RICHTER, K., and WULF, M.: The first stages of tenside layer formation. A metastable impact electron spectroscopy study of sodium oleate dissolved in formamide, **79**, 169
MORISHIGE, K., TAJIMA, Y., KITTAKA, S., CLARKE, S.M., and THOMAS, R.K.: The structure of cloromethane monolayers adsorbed on graphite, **72**, 395
MORISHIGE, K.: The structure of a monolayer film of carbon dioxide adsorbed on graphite, **78**, 1203
MORITA, TOHRU, TANAKA, KAZUYUKI and HIROIKE KAZUO: One-dimensional binary mixture of hard rods with non-additive distances of contact, **61**, 1549
MORO, G., *see* Coletta, F.
MORO, G., *see* Ferrarini, A.
MORO, G., NORDIO, P.L., and POLIMENO, A.: Multivariate diffusion models of dielectric friction and TICT transitions, **68**, 1131
MOROZOV, V.A., ANTZUTKIN, O.N., KOPTYUG, A.V., and DOKTOROV, A.V.: Multiquantum resonances in low-field optically detected ESR of radical-ion pairs, **73**, 517
MORRESI, A., *see* Döge, G.
MORRESI, A., *see* Giorgina, M.G.
MORRIS, A., *see* Barnes, M.
MORRISS, G.P., and KOK KEAN YIM: The Nosé bond constraint for diatomic molecules, **71**, 653
MORRISS, G.A., and SMITH, K.I.: Analysis of 'virtual one-bond coupling' effects in heteronuclear chemical shift correlation, 2D N.M.R. spectra, **61**, 467
MORRISS, G.P., *see* Edberg, R.
MORRISS, G.P., *see* Evans, D.J.
MORRISS, G.P., *see* Fraser, K.J.
MORRISS, G.P., *see* Hood, L.M.
MORRISON, G., *see* Mountain, R.D.
MORRISON, I.D., *see* Bartlett, J.M.
MORRISON, J.A., *see* Inaba, A.
MORTIMER, M., MOORE, E.A., APPERLY, D.C., and PIERSON, N.F.: Calculation of N.M.R. spin echo responses in solids containing both resonant and non-resonant spin-½ nuclei, **68**, 455
MOSINA, V.K., *see* Voronkova, V.K.
MOSKOWITZ, J.W., *see* Tawa, G.J.
MOSS, R.E.: Calculations for vibration-rotation levels of HD^+, in particular for high N, **78**, 371
MOSS, R.E.: Calculations for the vibration-rotation levels of H_2^+ in its ground and first excited electronic states, **80**, 1541
MOSS, R.E., *see* Kennedy, R.A.
MOSS, R.E., and SADLER, I.A.: Symmetry breaking effects in HD^+, **61**, 905
MOSS, R.E., and SADLER, I.A.: A transformed hamiltonian theory for HD^+ near dissociation, **64**, 165
MOSS, R.E., and SADLER, I.A.: Transformed hamiltonian theory for HD^+, **66**, 591
MOSS, R.E., and SADLER, I.A.: Variational calculations for high J, low v levels of HD^+, **68**, 1015
MOTTRAM, R.E., *see* Murrell, J.N.
MOU, CHUNG-YUAN, *see* Hse, Tze-Jeng
MOULE, G.A., *see* Attard, P.
MOULINASSE, S., *see* Dupont, G.
MOUNTAIN, R.D., *see* Guillot, B.
MOUNTAIN, R.D., and MORRISON, G.: Molecular dynamics study of liquid CCl_2F_2 and $CClHF_2$, **64**, 91

MOURITSEN, O.G., *see* Zhang, Z.
MOZE, O., *see* Ibberson, R.M.
MRUGALA, F.: Predissociation of the $D^1\Pi_u^+$ state of H_2 by photon impact, **65**, 377
MUELLER, K.T., *see* Cho, H.
MUENSTER, O., *see* Jokisarri, J.
MUENTER, J.S., *see* Randall, R.W.
MUGA, J.G., and LEVINE, R.D.: Dual ensemble and fluctuations for systems with random elements, **67**, 1209
MUGA, J.G., and LEVINE, R.D.: Spectral moments for systems described by an ensemble of hamiltonians, **67**, 1225
MÜLLEN, K., *see* Rautter, J.
MÜLLER, A., *see* Möller, D.
MÜLLER, A., *see* Stetter, M.
MÜLLER, A., WINKELMANN, J., BOUBLÍK, T., and FISCHER, J.: Mixtures of dipolar with nonpolar linear molecules. Results from simulations and theory, **78**, 121
MÜLLER, E.A., and GUBBINS, K.E.: Simulation of hard triatomic and tetratomic molecules. A test of associating fluid theories, **80**, 957
MÜLLER, E.A., and GUBBINS, K.E.: Triplet correlation function for hard sphere systems, **80**, 91
MULLER, M., *see* Guinet, Y
MULLER-DETHLEFS, K., *see* Attal-Trétout, B.
MUNN, R.W.: Invited Article. Electric dipole interactions in molecular crystals, **64**, 1
MUNN, R.W., *see* Fowler, P.W.
MUNOWITZ, M.: Exact simulation of multiple-quantum dynamics in solid-state NMR: implications for spin counting, **71**, 959
MURAD, S., and EVANS, D.J.: Heat induced polarization in molecular fluids, **69**, 697
MURAD, S., and EVANS, D.J.: Heat-induced polarization of molecular fluids, addendum, **80**, 219
MURAD, S., *see* Evans, D.J.
MURAD, S., *see* Kielpinski, A.L.
MURAD, S., *see* Mansour, K.A.
MURAD, S., *see* Powles, J.G.
MURAD, S., and POWLES, J.G.: The pressure second virial coefficient for vibrating homonuclear diatomic molecules, **67**, 495
MURAD, S., SETHI, D.P.S., and POWLES, J.G.: The pressure second virial coefficient of vibrating symmetric triatomic molecules, **71**, 297
MURAD, S., SINGH, D.P., HANLEY, H.J.M. and EVANS, D.J.: Thermal conductivity of a model diatomic fluid, **72**, 487
MURRAY, C.W., HANDY, N.C., and LAMING, G.J.: Quadrature schemes for integrals of density functional theory, **78**, 997
MURRAY, J.S., *see* Brinck, T.
MURRELL, J.N.: Long-range potentials of polyatomic molecular ions, **62**, 1403
MURRELL, J.N., *see* Al-Derzi, A.R.
MURRELL, J.N., *see* Belchior, J.C.
MURRELL, J.N., *see* Braga, J.P.
MURRELL, J.N., *see* Dunne, L.J.
MURRELL, J.N., *see* Eggen, B.R.
MURRELL, J.N., *see* Fang, J.-Y.
MURRELL, J.N., *see* Guo, H.
MURRELL, J.N., *see* Marks, A.J.
MURRELL, J.N., and MOTTRAM, R.E.: Potential energy functions for atomic solids, **69**, 571
MURRELL, J.N., and RODRIGUEZ-RUIZ, J.A.: Potential energy functions for atomic solids. II. Potential functions for diamond-like structures, **71**, 823
MURTHY, K., DHANARAJ, G., BHAT, H.L., and BHAT, S.V.: Electron paramagnetic resonance evidence for Jahn-Teller glasses, **65**, 181
MURUGESAN, R., THAMARAICHELVAN, A., FRANKLIN, A.M.,and RAMAKRISHNAN, V.: Host spin-lattice relaxation narrowing and the electron paramagnetic resonance of Mn(II) in single crystals of hexakis(pyridine *N*-oxide)cobalt(II) complexes, **79**, 663

MUSTAFA, M., *see* Maitland, G.C.
MUSTAFA, M., *see* McCourt, F.R.W.

NAARMANN, H., *see* Lang, A.
NABERUKHIN, Y.I., VOLOSHIN, V.P., and MEDVEDEV, N.N.: Geometrical analysis of the structure of simple liquids: percolation approach, **73**, 917
NABOKOV, O.A., and LUBIMOV, YU. A.: The dielectric relaxation and the percolation model of water, **65**, 1473
NACHMAN, D.F., *see* Steimle, T.C.
NAFIE, L.A., *see* Hecht, L.
NAGARATHNA-NAIK, H.M., *see* Ramondo, F.
NAGATA, R., KONDOW, T., and ZARE, R.N.: Fluorescence polarization of a diatomic fragment following photodissociation of a triatomic precursor, **70**, 1159
NAGY, J.B., *see* Decressain, R.
NAIDOO, K.J., SCHNITKER, J., and WEEKS, J.D.: Two-dimensional melting revisited. Molecular dynamics simulations initiated with optical microscopy data, **80**, 1
NAITO, S., FUKASE, S., TAKAGI, R., and KAWAMURA, K.: Examination of reference potentials for the molten $K_x(KCl)_{1-x}$ system by the Percus-Yevick approximation, **61**, 485
NAJIB, H., BENSARI-ZIZI, N., BURGER, H., GUELACHVILI, G., and ALAMICHEL, C.: Anharmonic resonances between the upper rovibrational levels of the $\upsilon_2 + \upsilon_4^{\pm 1}$, $N_2 + 3\upsilon_6^{\pm 1}$, $\upsilon_1 + \upsilon_5^{\pm 1}$, $3\upsilon_5^{\pm 1}$, $\upsilon_4^{\pm 1} + \upsilon_5^{\pm 1}$, $\upsilon_5^{\pm 1} + 3\upsilon_5^{\pm 1}$, $\upsilon_5^{\pm} 3\upsilon_6^{\pm 3}$ and $2\upsilon_3 + 3\upsilon_6^{\pm 1}$ infrared bands of $CH_3\,^{35}Cl$ studied in a high-resolution FTIR spectrum from 4250 to 4600 cm^{-1}, **70**, 849
NAJIB, H., SARI-ZIZI, N.G., GUELACHVILI, G., and ALAMICHEL, C.: Fourier transform high-resolution study of the $2\upsilon_4$ rovibrational band of $CH_3\,^{35}Cl$ from 5980 cm^{-1} to 6220 cm^{-1}, **79**, 747
NAKAI, T., ASHIDA, J., and TERAO, T.: Influence of small-amplitude motions on two-dimensional N.M.R. powder patterns. Anisotropic vibrations in calcium formate, **67**, 839
NAKAI, T., and MCDOWELL, C.A.: An analysis of NMR spinning sidebands of homonuclear two-spin systems using Floquet theory, **77**, 569
NAKAI, T., and MCDOWELL, C.A.: INADEQUATE NMR spectra of extremely strongly coupled spin systems, **79**, 965
NAKANISHI K., *see* Takamiya, M.
NAKAMURA, R., MACHIDA, K., OOBATAKE, M., and HAYASHI, S.: Molecular dynamics simulation of infrared spectra and average structure of benzoic acid crystal, **64**, 215
NAKANAGA, T., and AMANO, T.: High-resolution infrared identification of $HOCS^+$ with difference frequency laser spectroscopy, **61**, 313
NARASIMHAN, P.T., *see* Ramamoorthy, A.
NARASIMHAN, P.T., *see* Reddy, R.
NARDONE, M., *see* Benassi, P.
NARDONE, M., *see* De Santis, A.
NATANSON, G.A.: The Eckart-frame hamiltonian of a triatomic molecule in terms of the bond lengths and the intrabond angle, **66**, 129
NATANSON, G.A.: Wilson-Howard rotation-vibrational hamiltonian in the limiting case of a linear triatomic molecule, **67**, 173
NATTRASS, S.R., *see* McLauchlan, K.A.
NAUTS, A., *see* Chapuisat, X.
NAVASCUES, G., and TARAZONA, P.: A model for capillary crystallization and the capillary triple point, **62**, 49
NDIKUMANA, T., CARLEER, M., and COLIN, R.: Laser-induced fluorescence spectrum and radiative lifetimes of the gaseous PbSe molecule, **69**, 229
NEBOT-GIL, I., *see* Garcia-Guesta, I.
NEILSEN, G.W., *see* Adya, A.K.
NEILSON, G.W., *see* Howe, M.A.
NEILSON, G.W., *see* Powell, D.H.
NELIS, TH., BACHEM, E., BOHLE, W., and URBAN, W.: Vibration rotation spectroscopy of the NiH-radical in its $^2\Delta$-ground state by CO-Faraday-L.M.R., **64**, 759
NELIS, T., *see* Bachem, E.

NELIS, TH., *see* Lipus, K.
NELIS, TH., *see* Zimmermann, W.
NENCINI, L., SNELS, M., HOLLENSTEIN, H., and QUACK, M.: High-resolution spectra and analysis of the hot bands of the υ_2 vibration of $CF_3Cl(\upsilon_2 + \Pi_n - \upsilon_n, n = 3,5,6)$, **67**, 989
NEOH, K.G., *see* Kang, E.T.
NEUE, G., *see* Boddenberg, B.
NEUE, G., and BODDENBERG, B.: An N.M.R. study of an *n*-butane film of graphite. II. ^1H relaxation of the 2D fluid state, **68**, 771
NEUEFEIND, J., CHIEUX, P., and ZEIDLER, M.D.: Geometry and intermolecular structure of *N*-methylformamide in the liquid phase as measured by neutron scattering, **76**, 143
NEUGEBAUER, S.M., and TINTI, D.S.: Optical Zeeman and low-field ODMR studies of the $n\pi^*$ phosphorescence of *p*-chlorobenzaldehyde, **79**, 475
NEUMANN, M., *see* Hummer, G.
NEWMAN, D.J., and NG, B.: Intermediate symmetry, the superposition model and induced representations, **61**, 1443
NEWMARK, R.D., *see* Emsley, J.W.
NEWNHAM, D.A., *see* Baggott, J.E.
NEWNHAM, D.A., *see* Holland, J.K.
NEZBEDA, I., and IGLESIAS-SILVA, G.A.: Primitive model of water. III. Analytic theoretical results with anomalies for the thermodynamic properties, **69**, 767
NEZBEDA, I., *see* Kalyuzhny, Y.Y.
NEZBEDA, I., *see* Kolafa, J.
NEZBEDA, I., KOLAFA, J., and KALYUZHNYI, Y.V.: Primitive model of water. II. Theoretical results for the structure and thermodynamic properties, **68**, 143
NEZBEDA. I., *see* Labik, S.
NEZBEDA, I., RAMI REDDY, M., and SMITH, W.R.: Monte Carlo study of hard-body fluids at a hard wall: pure fluids and mixtures of spheres, heternuclear dumbbells and linear triatomics, **71**, 915
NEZBEDA, I., and SMITH, W.R.: Theory of the glass transition and the amorphous state. I. The hard-sphere fluid, **75**, 789
NEZBEDA, I., *see* Vörtler, H.L.
NG, B., *see* Newman, D.J.
NG, B., *see* Reid, M.F.
N'GOM, A., *see* Camy-Peyret, C.
NGUYEN, M.T.: Structures and energies of the two lowest-lying electronic states in the sulphido-borons radical cations, RBS^+ (R = H, F,Cl and CH_3), **62**, 735
NGUYEN, M.T., and GROARKE, P.J.: Calculated properties of some oxoborons R-B=0 (R = H, F, Cl and CH_3) and their higher energy isomers R-O=B, **75**, 1105
NGUYEN, M.T., VANQUICKENBORNE, L.G., PLISNIER, M., and FLAMMANG, R.: A mass spectrometric and *ab initio* molecular orbital characterization of thionitrosyl hydride (H-N=S), **78**, 111
NICKEL, B.S., *see* Basile, A.G.
NICKOLOV, ZH., *see* Zhelyaskov, V.
NICHOLS III, A.L., and CALEF, D.F.: Structure and thermodynamics of asymmetric molecules: Application to linear triatomic dipolar molecules, **71**, 169
NICHOLSON, D., *see* Cracknell, R.F.
NICHOLSON, D., *see* Parsonage, N.G.
NICOLAISEN, F.M., and NIELSEN, O.L.: SO_2 pressure broadening and frequency shifting of H_2O absorption lines in the infrared region, **62**, 1111
NICOLAISEN, H.-W., and MADER, H.: Rotational relaxation rates for the J = 0-1 transition of N_2O by self-collisions and foreign gas collisions, **73**, 349
NIEDZIELSKI, J., *see* Turulski, J.
NIELSEN, O.L., *see* Nicolaisen, F.M.
NIEPMANN, R., *see* Boddenberg, B.
NIJMEIJER, M.J.P., BRUIN, C., BAKKER, A.F., and VAN LEEUWEN, J.M.J.: A search for prewetting in a molecular dynamics simulation, **72**, 927
NIKIEL, L., *see* Bródka, A.

NIKIEL, L., WRZALIK, R., and BRÓDKA, A.: Temperature and pressure study of Fermi resonance spectrum in liquid benzene-h_6, **67**, 399

NIKITIN, E.E., REZNIKOV, A.I., and UMANSKII, S. YA.: Cross sections for charge exchange of atoms on multiple-charged ions. A comparative study of processes $Ar^{++}(3p^4)$, $Kr^{++}(4p^4)$ + $He(1s^2)$ → $Ar^+(3p^5)$, $Kr^+(4p^5)$ + $He^+(1s)$ in eV energy range, **65**, 1301

NIKITIN, E.E., and REZNIKOV, A.I.: Cross-sections for charge exchange of atoms on multiply charged ions. Charge exchange of $N^{2+}(1p)$ on $He(1s^2)$ in the eV energy range, **77**, 563

NILSSON, L.G., GULDBRAND, L., and NORDENSKIOLD, L.: Evaluation of the electrostatic osmotic pressure in an infinite system of hexagonally oriented DNA molecules. A Monte Carlo simulation study, **72**, 177

NILSSON, L.G., and PADRO, J.A.: A time-saving algorithm for generalized Langevin- dynamics simulations with arbitrary memory kernels, **71**, 355

NISHI, N., *see* Stace, A.J.

NIZAM, M., *see* Bouteiller, Y.

NOBES, R.H., *see* Tozer, D.J.

NOMURA, H., *see* Ohba, M.

NORDENSKIOLD, L., *see* Nilsson, L.G.

NORDIO, P.L., *see* Coletta, F.

NORDIO, P.L., *see* Ferrarini, A.

NORDIO, P.L., *see* Moro, G.J.

NORDIO, P.L., and POLIMENO, A.: Diffusion model for a reactive coordinate coupled to a solvent variable of different timescale, **75**, 1203

NORMAN, J.B., CROSS, K.J., SCHWEDA, H.S., POLAK, M., and FIELD, R.W.: The CaO $c^3\Sigma^+$ - $a^3\Pi_i(0,0)$ band. The key to the orange system and the global electronic structure of CaO, **66**, 235

NORO, M., *see* Variyar, J.E.

NORTH, A.N., *see* Calleja, M.

NORTHRUP, F.J., and SEARS, T.J.: Renner-Teller, spin-orbit and Fermi-resonance interactions in $X^2\Pi$ NCS investigated by LIF spectroscopy, **71**, 45

NOVARO, O., *see* Jarque, C.

NUYKEN, O., *see* Franzke, D.

NYBURG, S.C., and FAERMAN, C.H.: The role of bonding electrons in intermolecular forces; solid acetylene, **67**, 447

OBERBRODHAGE, J., *see* Morgner, H.

OBRIOT, J., *see* Guillot, B.

O'CONNELL, J.P., *see* Perry, R.L.

ODDERSHEDE, J., *see* Geertsen, J.

ODDERSHEDE, J., *see* Paidarova, I.

ODDERSHEDE, J., *see* Sauer, S.P.A.

ODELIUS, M., *see* Ribbing, C.

OELSCHLAGER, H., *see* Fischer, J.

OESCHLAGER, H., and SAAGER, B.: Angle averaged Boltzmann factor for hard dumb-bells, **62**, 429

OGILVIE, J.F., *see* Teffo, J.-L.

OGINO, Y., *see* Yamazaki, T.

OHASHI, K., *see* Stace, A.J.

OHBA, T., and IKAWA, S.: Far-infrared optical constants of liquid acetonitrile at 238 to 343K as measured with a synchrotron radiation source, **73**, 958

OHBA, T., and IKAWA, S.: Molecular dynamics study of local structure and reorientational dynamics in liquid acetonitrile, **73**, 999

OHBA, M., and NOMURA, H.: The second dielectric virial coefficient of non-ideal polar hard-sphere fluids and polar hard dumb-bell fluids, **65**, 1431

OHBA, M., and NOMURA, H.: The second dielectric virial coefficient of asymmetrical polar hard dumb-bell fluids, **70**, 729

OHBA, M., and NOMURA, H.: The dielectric constant and the site-site direct correlation function of the RISM-2 theory for polar polyatomic molecular fluids, **77**, 689
OHTORI, N., *see* Matsumoto, M.
OHYA-NISHIGUCHI, H, *see* Kouichi Fuykui
OJHA, P.C., and BERRY, R.S.: On adiabatic separation of stretching and bending vibrations, **63**, 909
OKADA, I., *see* Adya, A.K.
OKADA, I., *see* Matsumoto, M.
OKADA, I., *se* Okazaki, S.
OKADA, I., *see* Suzuki, Y.
OKAZAKI, S., MATSUMOTO, M., and OKADA, I.: Study of rotational and vibrational relaxation of the CO_3^{2-} ion in molten alkali carbonates by Raman spectroscopy, **79**, 611
OKAZAKI, S., *see* Adya, A.K.
OKAZAKI, S., *see* Matsumoto, M.
OKAZAKI, S., *see* Suzuki, Y.
OKSENGORN, B., *see* Lavorel, B.
OLDANI, M., *see* Jans-Berli, S.
OLIVIERI, A.C., *see* Frydman, L.
OLSSON, T., *see* Berg, L.-E.
O'MAHONY, J., *see* Brouard, M.
O'MARD, L., *see* Farman, H.
O'NAGIBTM H.M., *see* Brouard, M.
ONORI, G., *see* Petrillo, C.
OOBATAKE, M., *see* Katō, T.
OOBATAKE, M., *see* Nakamaura, R.
OPRZYNSKI, J., *see* Möller, D.
ORLANDO, R., *see* Salasco, L.
ORLIKOWSKI, , T., *see* Wolniewicz, L.
ORNELLAS, F.R., *see* Machado, F.B.C.
ORNELLAS, F.R., MACHADO, F.B.C., and ROBERTO-NETO, O.: A theoretical study of the molecules BeF and BeF^+ in their lowest-lying electronic states, **77**, 1169
OROZCO, J., *see* Castillo, R.
ORTEGA, J., *see* Récamier, J.
ORZA, J.M., *see* Santos
O'SHEA, S.F., *see* Dubey, G.S.
O'SHEA, S.F., *see* Rami Reddy, M.
OSHEROV, V.I., POLUYANOV, L.V., and BORONIN, A.I.: Quantum and semiclassical dynamics of quasilinear triatomic system near the adiabatic term intersection point of $\Sigma^+ = \Pi = \Sigma^-$ type, **66**, 1041
OSHTRAKH, M.I., SEMIONKIN, V.A., BURYKIN, B.N., and KHLESKOV, V.I.: Interpretation of Mössbauer spectra of deoxyhaemoglobin taking into account the non-equivalence of the Fe^{2+} electronic structure in different subunits, **66**, 531
OSIPOV, M.A., and HESS, S.: The elastic constants of nematic and nematic discotic liquid crystals with perfect local orientational order, **78**, 1191
OSS, S., *see* Iachello, F.
OSTAFIN, A., *see* Francisco, J.S.
OTTAVIANI, M.F., *see* Maniero, A.L.
OUAHMAN, M., SARI-ZIZI, N.B., GUELACHVILI, G., and ALAMICHEL, C.: Anharmonic resonances between the $\nu_1 + \nu_6^{\pm 1}$, $\nu_3 + \nu_5^{\pm 1} + 2\nu_6^0$ and $\nu_3 + \nu_5^{\mp 1} + 2\nu_6^{\pm 2}$ vibrational bands of $CH_3\,^{79}Br$, **76**, 1477
OUAZZANY, Y., BOQUILLON, J.P., and SCHROTTER, H.W.: High resolution CARS spectrum and analysis of the ν_1 band of the *Q*-branch of carbon dioxide, **63**, 769
OUILLON, R., *see* Le Duff, Y.
OUTHWAITE, C.W.: Image effects for point ions in a molecular solvent next to a plane wall, **63**, 77
OUTHWAITE, C.W., and BHUTYAN, L.B.: A modified Poisson-Boltzmann analysis of the electric double layer around an isolated spherical macroion, **74**, 367
OVCHINNIKOV, A.A., *see* Dakhnovskii, Yu. I.

OVERBEEK, J.T.G.: On the interaction of highly charged plates in an electrolyte: a correction, **80**, 685
OVSIANNIKOV, V.D., GUILYAROVSKI, A.V., and LOPATKO, O.YA .: Higher order effects in dispersion interaction of atoms, **64**, 111
OZAWA, S., *see* Yamazaki, T.
OZHOGINAO, O.A., *see* Rozantsev, E.G.
OACI, E., *see* Depaepe, J.-M.

PACIOS, L.F., *see* Walker, E.C.
PACKER, K.J., *see* Booth, A.D.
PACKER, M.J., and RAYNES, W.T.: Electric field effects on the ^{13}C and ^{19}F nuclear shielding in HF and CH_3F, **69**, 391
PADILLA, P., LAGO, S., and VEGA, C.: A bridge between Fischer and Boublik thermodynamic perturbation theories: calculating thermodynamic properties of pure substances, **74**, 161
PADRO, J.A., and CANALES, M.: Fractal analysis of atomic motions, **68**, 423
PADILLA, P., and TOXVÆRD, S.: Second virial coefficients of *n*-alkanes, **75**, 1143
PADRO, J.A., GUARDIA, E., and SESE, G.: On the use of effective memory functions in generalized Langevin dynamics simulation of interacting particles, **63**, 355
PADRO, J.A., *see* Nilsson, L.G.
PADRO, J.A.,. TRULLAS, J., and SESE, G.: Computer simulaton study of the dynamic cross-correlation in liquids, **72**, 1035
PAFF, J., and BLUMICH, B.: Nonlinear incoherent spectroscopy. Two-dimensional time-domain CW magnetic resonance, **68**, 225
PAGE, A.G., *see* Porwai, N.K.
PAHNKE, R., *see* Zimmermann, W.
PAIDAROVA, I., KOMASA, J., and ODDERSHEDE, J.: Correlated calculations for the nuclear magnetic shieldings of CO and HCN, **72**, 559
PAIS, A.A.C.C., *see* Varandas, A.J.C.
PALFFY-MUHORAY, P., *see* Dunmur, D.A.
PALIANI, G., *see* Giorgina, M.A.
PALII, A.V., *see* Tsukerblat, B.S.
PALINKAS, G., BAKO, I., HEINZINGER, K., and BOPP, P.: Molecular dynamics investigation of the inter- and intramolecular motions in liquid methanol and methanol-water mixtures, **73**, 897
PALMA, M.L., and BORDE, J.: Theoretical study of the rovibrational dependence of nuclear hyperfine interactions in the υ_3 band of SF_6, **70**, 863
PALMER, A.G., III, SKELTON, N.J., CHAZIN, W.J., WRIGHT, P.E., and RANCE, M.: Suppression of the effects of cross-correlation between dipolar and anisotropic chemical shift relaxation mechanisms in the measurement of spin-spin relaxation rates, **75**, 699
PALMERI, P., *see* Bearpark, M.J.
PANAGIOTOPOULOS, A.Z.: Direct determination of phase coexistence properties of fluids by Monte Carlo simulation in a new ensemble, **61**, 813
PANAGIOTOPOULOS, A.Z.: Adsorption and capillary condensation of fluids in cylindrical pores by Monte Carlo simulation in the Gibbs ensemble, **62**, 701
PANAGIOTOPOULOS, A.Z., *see* Recht, J.R.
PANAGIOTOPOULOS, A.Z., QUIRKE, N., STAPLETON, M., and TILDESLEY, D.J.: Phase equilibria by simulation in the Gibbs ensemble. Alternative derivation, generalization and application to mixture and membrane equilibria, **63**, 527
PANAGIOTOPOULOS, A.Z., *see* Woods, G.B.
PAOLINI, G.V., CICCOTTI, G., and FERRARIO, M.: Simulation of site-site soft-core liquid crystal models, **80**, 297
PAPOUSEK, D., *see* Sarka, K.
PAQUET, D.M., *see* McGuigan, D.B.
PARAS, E.P.A. VEGA, C., and MONSON, P.A.: Application of cell theory to the thermodynamic properties of hard dumbbell solids, **77**, 803
PARAS, E.P.A., VEGA, C., and MONSON, P.A.: A generalized van der Waals theory of solid-fluid equilibria for non-spherical molecules, **79**, 1063
PARBUZIN, V.S., *see* Larin, A.V.

PARDON, P.R., *see* Bell, A.J.
PARKIN, J.E., *see* Cossart-Magos, C.
PARRY, A.O., and EVANS, R.: Correlation functions in the approach to complete drying at a wall-liquid interface, **65**, 455
PARRY, A.O., and EVANS, R.: Fluctuations, correlation functions and interfacial Hamiltonians for the complete wetting phase transition, **78**, 1527
PARRY, A.O., *see* Evans, R.
PARSONAGE, N.G. *see* Cracknell, R.F.
PARSONAGE, N.G., and NICHOLSON, D.: A statistical mechanical study of a model for the stacking-unstacking behaviour of thylakoid membranes, **75**, 23
PARTRIDGE, H., *see* Shen, M.
PAS, M.F., and ZWOLINSKI, B.J.: Computation of the transport coefficients of dense fluid neon, argon, krypton and xenon by molecular dynamics, **73**, 471
PAS, M.F., and ZWOLINSKI, B.J.: Computation of the transport coefficients of binary mixtures of argon-krypton, krypton-xenon, and argon-xenon by molecular dynamics, **73**, 483
PASINI, P., *see* Biscarini, F.
PASINI, P., *see* Chiccoli, C.
PASMORE, T.A., *see* Courtemanche, D.J.
PASO, R., ALANKO, S., and ANTTILA, R.: Ground-state constants A_0, D_0^K *and* H_0^K of CH_3I from normally allowed infrared absorption bands, **76**, 1157
PASTOR, J.M., *see* Ferrero, F.S.
PASTOR, R.W., BROOKS, B.R., and SZABO, A.: An analysis of the accuracy of Langevin and molecular dynamics algorithms, **65**, 1409
PASTORE, G.: Uniqueness and the choice of the acceptable solutions of the MSA, **63**, 731
PASTORE, G., *see* Badirkhan, Z.
PASTORE, G., *see* Barrat, J.L.
PASTORE, G., and WAISMAN, E.M.: Structure of inverse-power fluids in analytical form, **61**, 849
PASTORE, G., and WAISMAN, E.M.: Structure of inverse-power fluids in analytical form (erratum), **63**, 351
PATERSON, C., *see* Godwin, F.G.
PATEY, G.N., *see* Caillol, J.M.
PATEY, G.N., *see* Kusalik, P.G.
PATEY, G.N., *see* Talbot, J.
PATEY, G.N., *see* Torrie, G.M.
PATRIARCA, M., *see* Gianturco, F.A.
PATRYKIEJEW, A., PENAR, J., and SOKOLOWSKI, S.: The second and third surface virial coefficient for hard dumb-bells in contact with a hard wall, **62**, 785
PAVLIDES, P., PUGH, D., and ROBERTS, K.J.: Elastic constants of molecular crystals in the pair-potential rigid-molecular approximation, **72**, 121
PAVLIDES, P., and CATLOW, C.R.A.: Elastic constants and lattice vibrations of CO_2 and C_6H_6, **79**, 1025
PAVLOV-VEREVKIN, V.B., *see* Desouter-Lecomte, M.
PAWLEY, G.S., *se* Craven, C.J.
PAWLEY, G.S., *see* Dove, M.T.
PAWLEY, G.S., *see* Powell, B.M.
PAWLEY, G.S., *see* Refson, K.
PAX, R., *see* Separovic, F.
PAYNE, M.P., *see* Cooper, .
PEIRSON, N.F., *see* Mortimer, M.
PELAN, E.G., *see* Dickinson, E.
PELISSIER, M., *see* Bouteiller, Y.
PELLOW, R., and VALA, M.: Magnetic circular dichroism and magnetic linear dichroism of randomly oriented linear molecules, **68**, 893
PENAR, J., *see* Patrykiejew, A.

PENFOLD, J., LEE, E.M., and THOMAS, R.K.: The structure of aqueous tetramethyl-ammonium dodecylsulphate solutions at the air-water interface studied by the specular reflection of neutrons, **68**, 33

PENFOLD, J., *see* Li, Z.X.

PENG, W.-G., STRAUSS, M., PIEPER, T., and KILIAN, H.-G.: X-ray diffraction and model calculation on carbon blacks, **80**, 419

PENOTTI, F., *see* Walters, S.G.

PEPLINSKA, B., *see* Andrew, E.R.

PERCUS, J.K., and ZHANG, M.Q.: The quasi-one dimensional hard square gas, **69**, 347

PERERA, A., *see* Talbot, J.

PERERA, A., *see* Torrie, G.M.

PEREZ, J., *see* Calvo Hernández, A.

PEREZ, J., *see* Velasco, S.

PERGAMENSHCIK, V.M., *see* Teixeira, P.I.C.

PERIĆ, M., BHANUPRAKASH, K., and BUENKER, R.J.: *Ab initio* MRD-CI study of the Renner-Teller effect and spin-orbit coupling in the X $^2\Pi_g$ ground state of BO_2, **65**, 403

PERIĆ, M., BUENKER, R.J., and PEYERIMOFF, S.D.: Theoretical study of the vibronic structure of the 1 $^1\Pi \leftarrow X\ ^1\Sigma^+$ electronic transition in HCN and DCN, **62**, 1323

PERIĆ, M., BUENKER, R.J., and PEYERIMHOFF, S.D.: *Ab initio* CI study of the vibrational structure of the 1 $^1\Sigma^-$ (1 $^1A''$) $\leftarrow X$ and 1 $^1\Delta$ (2 $^1A'$, 2 $^1A''$) $\leftarrow X$ electronic transitions in HCN and DCN, **64**, 843

PERIĆ, M., BUENKER, R.J., and PEYERIMHOFF, S.D.: *Ab initio* investigation of the vibronic structure of the C_2H spectrum. II. Calculation of diabatic potential surfaces for the three lowest-lying electronic states in C_2H, **71**, 673

PERIĆ, M., PEYERIMHOFF, S.D., and BUENKER, R.J.: Theoretical study of the U.V. spectrum of acetylene. III. *Ab initio* investigation of the valence-type singlet electronic states, **62**, 1339

PERIĆ, M., PEYERIMHOFF, S.D., and BUENKER, R.J.: *Ab initio* investigation of the vibronic structure of the C_2H spectrum. III. Calculation of vibronic energies and transition probabilities in the $X^2\Sigma^+$, $A^2\Pi$ system, **71**, 693

PERIĆ, M., and PEYERIMHOFF, S.D.: *Ab initio* CI investigation of the electronic spectrum of BF_2. I. Calculation of the potential surfaces and the transition moments for the valence and Rydberg doublet electronic states, **78**, 855

PERIĆ, M., and PEYERIMHOFF, S.D.: *Ab initio* CI investigation of the electronic spectrum of BF_2. II. Interpretation and prediction of features of the 1^2A_1, -1^2B_1, 2^2A_1 absorption and emission, system, **78**, 877

PERIĆ, M., *see* Reuter, W.

PERIĆ, M., *see* Staikova, M.

PERKOVIĆ, S., SZLEIFER, I., and WIDOM, B.: Structure and tension of the boundary between surface phases, **80**, 729

PERKYNS, J.S., *see* Caillol, J.M.

PERLY, B., *see* Baldo, M.

PERRAM, J.W., *see* Petersen, H.G.

PERRAM, J.W., and PETERSEN, H.G.: Algorithms for computing the dynamical trajectories of flexible bodies, **65**, 861

PERRAM, J.W., PETERSEN, H.G., and DE LEEUW, S.W.: An algorithm for the simulation of condensed matter which grows and the $^3/_2$ power of the number of particles, **65**, 875

PERRAM, J.W., and PRAESTGAARD , E.: Perturbation theory for molecular fluids using a hard ellipsoid reference system, **63**, 1103

PERRAM, J.W., RASMUSSEN, J., and PRAESTGAARD, E.: On the determination of effective hard convex body parameters for liquid mixtures, **64**, 617

PERRIN, A., FLAUD, J.-M., CAMY-PEYRET, C., CARLI , B., and CARLOTTI, M.: The far infrared spectrum of $^{14}N^{16}O_2$. Electron spin-rotation and hyperfine Fermi contact resonances in the ground state, **63**, 791

PERRIN, A., LADO-BORODOWSKY, O., and VALENTIN, A.: The υ_3 and υ_4 interacting bands of HNO_3 line positions and line intensities, **67**, 249

PERROT, J.P., FEMELAT, B., BROYER, M., and CHEVALEYRE, J.: Ω doubling in 1_g state and electronic transition for BO_u^+ towards O_g^+ and $1_g(^3P_2)$ states of iodine, **61**, 97

PERROT, J.P., FEMELAT, B., SUBTIL, J.L., BROYER, M., and CHEVALEYRE, J.: Electronic transitions moments from both fluorescence intensities and lifetime measurements for transitions involving the I_2 ionic states, **61**, 85

PERROT, M., *see* Bouachir, M.

PERRY, R.L., CABEZAS, H., and O'CONNELL, J.P.: Fluctuation thermodynamic properties of strong electrolyte solutions, **63**, 189

PESTELLI, S., *see* Bafile, U.

PETERS, C.J., *see* Cornelisse, P.M.W.

PETERSEN, H.G., DE LEEUW, S.W., and PERRAM, J.W.: Applied field simulations of Stockmayer fluids, **66**, 637

PETERSEN, H.G., and PERRAM, J.W.: Molecular dynamics of transputer arrays. I. Algorithm design, programming issues, timing experiments and scaling projections, **67**, 849

PETERSEN, H.G., *see* Perram, J.W.

PETERSEN, J.C., *see* Hettner, W.

PETERSON, B.K., and GUBBINS, K.E.: Phase transitions in a cylindrical pore. Grand canonical Monte Carlo, mean field theory and the Kelvin equation, **62**, 215

PETRI, J., *see* Castillo, R.

PETRI, M., *see* Huhn, B.

PETRI, M., *see* Simon, U.

PETRI, M., SIMON, U., ZIMMERMANN, W., URBAN, W., TOWLE, J.P., and BROWN, J.M.: Infrared diode laser spectroscopy of the ground state of GeH ($X^2\Pi_{3/2}$), **72**, 315

PETRILLO, C., *see* Andreani, C.

PETRILLO, C., *see* Bellissent-Funel, M.-C.

PETRILLO, C., *see* Ibberson, R.M.

PETRILLO, C., ONORIE, G., and SACCHETTI, F.: Hydration structure of ethanol water solution at low alcohol concentrations, **67**, 697

PETRONGOLO, C., HIRSCH, G., and BUENKER, R.J.: Diabatic representation of the $\tilde{A}^2A_1/B^2B_2$ conical intersection in NH_2, **70**, 825

PETRONGOLO, C., *see* Hirsch, G.

PETRY, W., *see* Besnard, M.

PETRY, W., *see* Guillaume, F.

PETSALAKIS, I.D., *see* Theodorakopoulos, G.

PETSALAKIS, I.D., THEODORAKOPOULOS, G., and CONSTA, S.: Theoretical calculations on the electronic state of XeH, **75**, 805

PETTITT, B.M., *see* Çağin, T.

PETTITT, B.M., *see* Madura, J.D.

PEYERIMHOFF, S.D., *see* Anglada, J.

PEYERIMHOFF, S.D., *see* Banichevich, A.

PEYERIMHOFF, S.D., *see* Daskalopoulou, M.

PEYERIMHOFF, S.D., *see* de Vivie, R.

PEYERIMHOFF, S.D., *see* Engels, B.

PEYERIMHOFF, S.D., *see* Hippe, D.

PEYERIMHOFF, S.D., *see* Karna, S.P.

PEYERIMHOFF, S.D., *see* Matsushita, T.

PEYERIMHOFF, S.D., *see* Perić, M.

PEYERIMHOFF, S.D., *see* Reuter, W.

PEYERIMHOFF, S.D., *see* Staikova, M.

PFAB, J., *see* Harper, P.G.

PHILLIPS, C.R., *see* Busigin, A.

PHILLPOT, S.R., and RICKMAN, J.M.: Temperature dependence of the thermodynamic properties of a liquid over a wide range of temperatures from simulations at a single temperature, **75**, 189

PHIPPEN, R.W., *see* Adams, D.J.

PHOTINOS, D.J., JANIK POLIKS, B., SAMULSKI, E.T., TERZIS, A.F., and TORIUMI, H.: n-Hexane proton dipolar couplings and the rotational isomeric state approximation, **72**, 333

PIASECKI, J., *see* Szamel, G.
PICARD, A., *see* Aroui, H.

PICARD-BERSELLINI, A., *see* Broquier, M.
PICCIRILLO, S., *see* Hollenstein, H.
PICKUP, B.T., *see* Cook, D.B.
PIECUCH, P.: Spherical tensor theory of long-range interactions in a system of N arbitrary molecules including quantum-mechanical many-body effects, **66**, 805
PIELA, L., *see* Gutowski, M.
PIEPER, J., *see* Straty, G.C.
PIEPER, T., *see* Peng, W.-G.
PIERRE, G., *see* Tyuterev, V.G.
PIERRUS, J., *see* Graham, C.
PIERLEONI, , C., and RYCKAERT, J.-P.: On the use of the Nosé-Hoover thermostat in the simulation of dynamic properties of a single chain molecule in solvent, **75**, 731
PIKE, C.G., *see* Pyper, N.C.
PIKKEMAAT, J.A., *see* Gribnau, M.C.M.
PILLING, M.J., *see* Green, N.J.B.
PIMBLOTT, S.M., *see* Green, N.J.B.
PINAN-LUCARRE, J.P., *see* Dayan, E.
PINERO, P., *see* Velarde, J.M.
PINES, A., *see* Cho, H.
PINES, A., *see* Gochin, M.
PINES, A., *see* Luzar, M.
PINES, A., *see* Samoson, A.
PINES, A., *see* Suter, D.
PINNAVAIA, N., BRAMLEY, M.J., SU, M.-D., GREEN, W.H., and HANDY, N.C.: A study of the ground electronic state of the isomers of CHNO, **78**, 319
PINZINO, C., *see* Colligiani, A.
PIPIN, J., *see* Bishop, D.M.
PITTMAN, M., *see* Broquier, M.
PITZER, R.M., *see* Häussermann, U.
PIZIO, O.: On the simple derivation of approximate integral equations for triplet and higher-order distribution functions of homogeneous fluids, **77**, 1011
PLATO, M., *see* Jaegermann, P.
PLISCHKE, M., *see* Henderson, D.
PLISNIER, M., *see* Nguyen, M.T.
POGODA, M., *see* Powles, J.G.
POLAK, M., GRUEBELE, M., DEKOCK, B.W., and SAYKALLY, R.J.: Velocity modulation infrared laser spectroscopy of molecular ions. The υ_4 band of ammonium, **66**, 1196
POLAK, M., *see* Norman, J.B.
POLAK, R., and KUNTZ, P.J.: On the fragment input calculation for the diatomics-in-molecules method. Application to H_2O, **63**, 865
POLAK, R., and VOJTIK, J.: Diatomics-in-molecules treatment of NH_3, **68**, 447
POLAVARAPU, P.L., *see* Barron, L.D.
POLIMENO, A., *see* Moro, G.J.
POLIMENO, A., *see* Nordio, P.L.
POLINGER, V.Z., *see* Bersuker, G.I.
POLITOWICZ, P.A., and KOZAK, J.J.: Influence of channel geometry on sorption in zeolites, **62**, 939
POLITZER, P., *see* Brinck, T.
POLL, J.D., *see* Basile, A.G.
POLL, J.D., *see* Dore, P.
POLL, J.D., *see* Wolniewicz, L.
POLUEKTOV, O.G., *see* Bresgunov, A.Yu.
POLUYANOV, L.V., *se* Aguilar, A.
POLUYANOV, L.V., *see* Osherov, V.I.

PONIEWIERSKI, A., *see* Holyst, R.
PONIEWIERSKI, A., and SLUCKIN,, T.J.: Nematic, Smectic-A, and Smectic-C ordering in a system of parallel cylinders with quadrupolar interaction, **73**, 199
POPLE, J.A., *see* Tozer, D.J.
POPOV, A.F., *see* Vetchinkin, S.I.
PORCHER, P., *see* Bailleul, S.
PORWAL, N.K., SASTRY, M.D., GODBOLE, S.V., and PAGE, A.G.: ESR and TSL studies of gamma-irradiated $K_2UO_2(SO_4)_2.2H_2$) and $Rb_2UO_2(SO_4).2H_2O$, **72**, 295
POSCH, H.A., *see* Vesely, F.J.
POSHUSTA, R.D., SCHMALZ, T.G., and KLEIN, D.J.: Heisenberg-model cluster expansion for half-filled Hubbard and PPP models, **66**, 317
POSPÍŠIL, R., *see* Labik, S.
POSPÍŠIL, R., *see* Malijevský, A.
POSPÍŠIL, R., and MALIJEVSKÝ, A.: Integral equation study of hard sphere fluids near a hard cylinder macromolecule, **76**, 1423
POSPÍŠIL, R., MALIJEVSKÝ, A., and LABÍK, S.: Effect of three-body interactions on third virial coefficients of rare gases, **64**, 21
POSPISIL, R., MALIJEVSKÝ, A., and LABÍK, S.: An integral equation method for quadrupolar hard dumbbell fluids, **68**, 609
POSPISIL, R., MALIJEVSKÝ, A., LABÍK, S., and SMITH, W.R.: An accurate integral equation for molecular fluids. III. Hard linear homonuclear triatomics, **74**, 253
POSPÍŠIL, R., SÝS, J., MALIJEVSKÝ, A., and LABÍK, S.: Monte Carlo study of hard sphere fluids near a hard cylinder macromolecule, **75**, 261
POSPÍŠIL, R., MALIJEVSKÝ, A., JECH, P., and SMITH, W.R.: Integral equation and computer simulation studies of hard spheres in a slit pore, **78**, 1461
POSPÍŠIL, R., MALIJEVSKÝ, A., and SMITH, W.R.: An accurate integral equation for molecular fluids. V. Hard prolate ellipsoids of revolution, **79**, 1011
POSTORINO, P., *see* Andreani, C.
POSTORINO, P., *see* Filabozzi, A.
POUWELS, P.J.W., *see* Huis, L.
POWELL, B.M., *see* Bartell, L.S.
POWELL, B.M., DOVE, M.T., PAWLEY, G.S., and BARTELL, L.S.: Orientational ordering and the lower temperature structure of SF_6 , **62**, 1127
POWELL, B.M., *see* Dove, M.T.
POWELL, B.M., *see* Ikram, A.
POWELL, B.M., *see* Torrie, B.H.
POWELL, B.M., *see* Prystupa, D.A.
POWELL, B.M., *see* Weng, S.-X.
POWELL, D.H., GULLIDGE, P.M.N., NEILSON, G.W., and BELLISSENT-FUNELL, M.C.: Zn^{2+} hydration and complexation in aqueous electrolyte solutions, **71**, 1107
POWLES, J.G.: A model for atomic and molecular motion in liquids, **67**, 1021
POWLES, J.G., DAVIS, C., EVANS, W.A.B., and MURAD, S.: Diffusion in vibrating-molecule liquids, **70**, 529
POWLES, J.G., and FOWLER, R.F.: A simple property of a simple liquid, **62**, 1079
POWLES, J.G., and FOWLER, R.F.: Finite fractal analysis for Lennard-Jones liquids, **62**, 1085
POWLES, J.G., *see* Calleja, M.
POWLES, J.G., *see* Heyes, D.J.
POWLES, J.G., *see* Mansour, K.A.
POWLES, J.G., *see* Murad, S.
POWLES, J.G., MURAD, S., SETHI, D.P., and RAVI, P.V.: On the solvent frequency shift, **73**, 1307
POWLES, J.G., and POGODA, M.: A flexible model for the simulation of fluids in infinite porous systems, **78**, 757
POWLES, J.G., RICKAYZEN, G., and FOWLER, R.F.: Finite fractal analysis for finite trajectories in fluids, **61**, 887
POWLES, J.G., RICKAYZEN, G., and WILLIAMS, M.L.: The density profile of a fluid confined to a slit, **64**, 33

POWLES, J.G., WILLIAMS, M.L., and EVANS, W.A.B.: The dynamic dielectric constant of an inhomogeneous polar liquid: direct approach from simulation, **66**, 1107
PRAESTGAARD, E., *see* Perram, J.W.
PRAET, M. TH., *see* Desoute-Lecomte, M.
PRANDOLINI, M.J., *see* Bowden, G.J.
PRAUSNITZ, J.M., *see* Smit, B.
PRESTON, S.R., *see* Gardner, P.J.
PRESUNKA, P.I., *see* Coxon, J.A.
PREUSS, H., *see* Bergner, A.
PREUSS, H., *see* Dolg, M.
PREUSS, H., *see* Häussermann, U.
PREUSS, H., *see* Ingel-Mann, G.
PREUSS, H., *see* Küchle, W.
PREUSS, H., *see* Igel-Mann, G.
PREVOST, M., VAN BELLE, D., LIPPENS, G., and WODAK, S.: Computer simulations of liquid water: treatment of long-range interactions, **71**, 587
PRICE, A.H., *see* Guillaume, F.
PRICE, D.L., *see* Saboungi, M.-L.
PRICE, S.L.: The structure of the homonuclear diatomic solids revisited. A distorted atom approach to the intermolecular potential, **62**, 45
PRICE, S.L., *see* Wheatley, R.J.
PRICE, S.L., *see* Yashonath, S.
PRICE, W.E., *see* Harris, K.R.
PRIELMEIER, F.X., *see* Speedy, R.J.
PRIETO, C., *see* Chahid, A.
PRINCE, J.D., *see* Ashfold, M.N.R.
PRINGLE, W.C., COHEN, R.C., and JACOBS, S.M.: Analysis of collision induced far infrared spectrum of ethylene, **62**, 661
PRINGLE, W.C., GRONLUND, W.R., and COHEN, R.C.: Collision induced far infrared spectrum of cyclopropane, **62**, 669
PRITCHARD, H.O., *see* Shen, D.
PROKOF'EV, A.I., *see* Bresgunov, A. Yu.
PROKOF'EV, A.I., *see* Rozantsev, E.G.
PROUTIERE, A.: Agreement between molecular polarizability anisotropies (γ^2) deduced from Rayleigh light scattering and static Kerr birefringence in liquids - experimental and theoretical aspects, **65**, 499
PRYSTUPA, D.A., TORRIE, B.H., POWELL, B.M., and GERLACH, P.N.: Crystal structures of methylene bromide and methylene iodide, **68**, 835
PUGH, D., *see* Pavlides, P.
PULAY, P., *see* Van Lenthe, J.H.
PULKKINEN, O., *see* Jokisarri, J.
PUSEY, P.N., and RARITY, J.G.: Measurement of the hydrodynamic fractal dimension of aggregating polystyrene spheres, **62**, 411
PYKA, J.: Clustering of rovibrational energy levels in the highly excited H_2S molecule, **70**, 547
PYKA, J., *see* Makarewicz, J.
PYPER, N.C.: Exact relativistic analogues of the non-relativistic hyperfine structure operators. I. Theory, **64**, 933
PYPER, N.C., *see* Edwards, P.P.
PYPER, N.C., PIKE, C.G., and EDWARDS, P.P.: The polarizabilities of species present in ionic solutions, **76**, 353
PYPER, N.C., *see* Zhang, Z.C.
PYYKKO, P.: *Ab initio* study of bonding trends among the 14-electron diatomic systems: from B_2^{4-} to F_2^{4+}, **67**, 871
PYYKKO, P., GORLING, A., and ROSCH, N.: A transparent interpretation of the relativistic contribution to the N.M.R. 'heavy atom chemical shift', **61**, 195

PYYKKO, P., and YONGFANG ZHAO: *Ab initio* study of bonding trends 6. The X≡Y and X≡Y≡Z species containing phosphorus, **70**, 701

QUACK, M., *see* Hollenstein, H.
QUACK, M., *see* Luckhaus, D.
QUACK, M., *see* Nencini, L.
QUACK, M., *see* von Puttkamer, K.
QUACK, M., *see* Ross, A.J.
QUACK, M., *see* Snells, M.
QUACK, M., and SUHM, M.A.: Potential energy surface and energy levels of $(HF)_2$ and its D isotopomers, **69**, 791
QUANTIN, V.M., *see* Hills, B.P.
QUELCH, G.E., XIE, Y., YATES, B.F., YAMAGUCHI, Y., and SCHAEFFER III, H.F.: The HO_2^+ ion. A comparison of theoretical methods for the prediction of anharmonic vibrational frequencies, **68**, 1095
QUINTELLA, C.M., *see* Kenyon, A.J.
QUIRKE, N., *see* Cracknell, R.F.
QUIRKE, N., *see* Panagiotopoulos, A.Z.
QUIST, P.-O., and HALLE, B.: N.M.R. lineshapes from quadrupolar nuclei in biaxial lyotropic structures. Elliptic rod with nonuniform molecular distribution and orientational order, **65**, 547

RAAB, R.E., *see* Graham, C.
RAAB, R.E., *see* Imrie, D.A.
RAEDT, E., *see* Harris, K.R.
RAI, S.N., *see* Jensen, P.
RAIMONDI, M., *see* Raos, G.
RAINERI, F.O., and FRIEDMAN, H.L.: Determination of the mutual-diffusion coefficient of a binary mixture by non-equilibrium molecular dynamics viewed as a sedimentation experiment, **70**, 209
RAKHIMOV, R.R., *see* Rozantsev, E.G.
RAKVIN, B., KAHOL, P.K., and DALAL, N.S.: Electron nuclear double resonance near the phase transitions of the KH_2PO_4-type of ferroelectrics, **68**, 1185
RACZYNSKI, A.: Quantum-mechanical collision-induced absorption spectrum - Mori approach, **63**, 1095
RADLOFF, C., and ERNST, R.R.: Spin topology filtration in N.M.R., **66**, 161
RAEYMAEKERS, P., FIGEYS, H.P., and GEERLINGS, P.: *Ab initio* calculations of static dipole polarizabilities using improved virtual orbitals and symmetry adapted polarization functions. I. Theory and the H_2O case study, **65**, 925
RAEYMAEKERS, P., FIGEYS, H.P., and GEERLINGS, P.: *Ab initio* calculations of static dipole polarizabilities using improved virtual orbitals and symmetry adapted polarization functions. II. Application to polyatomic molecules, **65**, 945
RAIMBAUD, E.R., *see* Belton, P.S.
RAIMONDI, M., *see* Barnard, S.A.
RAIMONDI, M., *see* Sironi, M.
RAIMONDI, M., *see* Walters, S.G.
RAMAKRISHNAN, V., *see* Murugesan, R.
RAMAMOORTHY, A.: Double quantum nuclear quadrupole resonance spectroscopy of spin $I = 7/2$ nuclei in zero magnetic field, **72**, 1425
RAMAMOORTHY, A., and NARASIMHAN, P.T.: Broadband excitation sequences for NQR spectroscopy, **73**, 207
RAMASESHA, S., ALBERT, I.D.L., and SINHA, B.: Optical and magnetic properties of the exact PPP states of biphenyl, **72**, 537
RAMASWAMY, R., *see* Sinha, S.
RAMI REDDY, M., *see* Nezbeda, I.

RAMI REDDY, M., SWAMY, K.N., and O'SHEA, S.F.: Structure of liquid metals. Monte Carlo and integral equation perturbation theory, **62**, 333

RAMONDO, F., and BENCIVENNI, L.: *Ab initio* calculations on SO_2^- and the $NaSO_2$ charge transfer complex, **67**, 707

RAMONDO, F., BENCIVENNI, L., ROSSI, V., and NAGARATHNA-NAIK, H.M.: FTIR spectra of matrix isolated group 1*a* metal sulphates, **64**, 1145

RAMONDO, F., ROSSI, V., and BENCIVENNI, L.: Structure and vibrational frequencies of CaF_2 agregates isolated in a low temperature matrix, **64**, 513

RAMSAY, D.A., *see* Hettner, W.

RANCE, M., *see* Palmer, A.G. III.

RANDALL, R.W., CLIFFE, A.J., HOWARD, B.J., and MCKELLAR, A.R.W.: The infrared spectrum of Ne-CO. Analysis of combined jet and static cell data for ^{20}Ne and ^{22}Ne, **79**, 113

RANDALL, R., WILKIE, J.M., HOWARD, B.J., and MUENTER, J.S.: Infrared vibration-rotation spectrum and structure of OCS dimer, **69**, 839

RAOS, G., GERRATT, J., COOPER, D.L., and RAIMONDI, M.: On the role of different spin bases within spin-coupled theory, **79** 197

RARITY, J.G., *see* Pusey, P.N.

RASMUSSEN, J., *see* Perram, J.W.

RASSAT, A., *see* André, D.

RATAICZAK, R.D., *see* Maruo, T.

RATKJE, S.K., *see* Hafskjold, B.

RAUTTER, J., GRUPP, A., MEHRING, M., ALEXANDER, J. MÜLLEN, K., and HUBER, W.: Electron localization and delocalization in biselectrophores, **76**, 37

RAVI, P.V., *see* Powles, J.G.

RAVI KUMAR, R., LINGHAM, K.V., and GUNDU RAO, T.K.: ESR and proton ENDOR studies in single crystals of ammonium hydrogen l-malate, **72**, 1299

RAVISHANKAR, V.R.: Spin 1 and 3/2 systems in quadrupole fields, **62**, 1409

RAY, A.K., *see* Golden, K.I.

RAY, J.R., *see* Graben, H.W.

RAYANE, D., *see* Broyer, M.

RAYBONE, D., *see* Lindberg, P.

RAYNES, W.T.: Theory of vibrational effects on properties of methane and its isotopomers. The polarizability, magnetizability, carbon-13 shielding and the one- and two-bond spin-spin coupling constants, **63**, 719

RAYNES, W.T., *see* Bennett, B.

RAYNES, W.T., FOWLER, P.W., LAZZERETTI, P., ZANASI, R., and GRAYSON, M.: The effects of rotation and vibration on the carbon-13 shielding, magnetizabilities and geometrical parameters of some methane isotopomers, **65**, 143

RAYNES, W.T., *see* Lazzeretti, R.

RAYNES, W.T., LAZZERETTI, R., and ZANASI, R.: Theory of the carbon-13 proton spin-spin coupling and the proton shielding surfaces of the methane molecule, **61**, 1415

RAYNES, W.T., LAZZERETTI, R., and ZANASI, R.: Vibration-rotation effects on the polarizabilities of CH_4 and CD_4 calculated from an *ab initio* polarizability surface, **64**, 1061

RAYNES, W.T., *see* Packer, M.J.

REATTO, L., *see* Meroni, A.

RECAMIER., J. and BERRONDO, M.: Vibration-translation energy transfer in a collision between an atom and a Morse oscillator, **73**, 831

RECAMIER, J.and ORTEGA, J.: Transition probabilities in collisions between an atom and an anharmonic oscillator, **73**, 635

RECHT, J.R., and PANAGIOTOPOULOS, A.Z.: Finite-size effects and approach to criticality in Gibbs ensemble simulations, **80**, 843

REDDY, R., and NARASIMHAN, P.T.: Application of tensor operator formalism in pulsed nuclear quadrupole resonance spectroscopy. Part 1: Spin $I = {}^3/_2$ case in zero field, **72**, 491

REDDY, R., and NARASIMHAN, P.T.: Application of tensor operator formalism in pulsed nuclear quadrupole resonance spectroscopy. Part 1: Spin $II = {}^3/_2$ case in a weak Zeeman field, **72**, 509

REFSON, K., and PAWLEY, G.S.: Molecular dynamics studies of the condensed phases of n-butane and their transitions. I. Techniques and model results, **61**, 669

REFSON, K., and PAWLEY, G.S.: Molecular dynamics studies of the condensed phases of n-butane and their transitions. II. The transition to the true plastic phase, **61**, 693

REH, M., RÖDER, M., and VERSMOLD, H.: Depolarized Rayleigh and Raman scattering from N_2. Experimental verification of a neglected broadening/narrowing mechanism for rotation-vibration bands in fluids, **80**, 407

REHAGE, H., and HOFFMAN, H.: Visoelastic surfactant solutions: model systems for rheological research, **74**, 933

REID, M.F., *see* Jayasankar, C.K.

REID, M.F., *see* May, P.S.

REID, M.F., and NG, B.: Complete second-order calculations of intensity parameters for one-photon and two-photon transitions of rare-earth ions in solids, **67**, 407

REIHL, B., *see* Magnusson, K.O.

REIJERSE, E.J., *see* Van der Pol, A.

REIS, H., *see* Rodrigues, S.V.

REISS, H., *see* Speedy, R.J.

REISSE, J., *see* Luhmer, M.

REMEROWSKI, M.L., GLASER, S.J., and DROBNY, G.P.: A theoretical study of coherence transfer by isotropic mixing. Calculation of pulse sequence performance for systems of biological interest, **68**, 1191

REMLER, D.K., and MADDEN, P.A.: Invited Article. Molecular dynamics without effective potentials via the Car-Parrinello approach, **70**, 921

RENDELL, A.P., *see* Hirst, D.M.

RENNIE, A.R., *see* Li, Z.X.

REQUENA, A., ZUNIGA, J., FRANCES, J.M., and HIDALGO, A.: Perturbative calculation of energy levels for coupled oscillators using the adiabatic approximation, **61**, 1513

RESHETNYAK, V.V., *see* Kuyshinksky, N.G.

REUTER, W., PERIĆ, M., and PEYERIMHOFF, S.: *Ab intio* study of the vibronic structure for the X^2B_1 and A^2a_1 electronic states of H_2O^+, **74**, 569

REY, C., *see* Gallego, L.J.

REY, P., *see* Belorizky, E.

REYES, O., *see* Fuentealba, P.

REY-LAFON, M., *see* Guillaume, F.

REYNHARDT, E.C., *see* Fenrych, J.

REYNHARDT, E.C.: An NMR, DSC and X-ray investigation of the disaccharides sucrose, maltose and lactose, **69**, 1083

REYNHARDT, E.C.: An NMR investigation of proton transfer dynamics in solid naphthazarin B and C, **76**, 525

REYNHARDT, E.C., and FRONEMAN, S.: ^1H, ^{23}Na, and ^{21}P N.M.R. in the disodium salt of glucose 1-phosphate, **66**, 921

REYNHARDT, E.C., and FRONEMAN, S.: Phase transitions and molecular motions in crystalline *ortho*- and *meta*-carborane, **74**, 61

REYNHARDT, E.C., JURGA, S., and JURGA, K.: The structure and molecular dynamics of solid *n*-decylammonium chloride, **77**, 257

REYNOLDS, C.A., KING, P.M., and RICHARDS, W.G.: Free energy calculations in molecular biophysics, **76**, 251

REYNOLDS, P.A., *see* Day, P.

REYNOLDS, P.A., *see* Figgis, B.N.

REZNIKOV, A.I., *see* Nikitin, E.E.

RHYKERD, C.L., JR., *see* Schoen, M.

RHYKERD, C.L., *see* Shaoyi Jiang

RIBBING, C., ODELIUS, M., and KOWALEWSKI, J.: Simple nonempirical calculations of the zero field splitting in transition metal systems. II. NiF_6^{4-} and Ni(II) complexes with mixed ligands, **74**, 1299

RIBBING, C., and ODELIUS, M.: Normal coordinate analysis of the zero-field splitting in octahedral NiF_6^{4-}. I. *Ab initio* calculations, **78**, 1259

RICCI, F.P., *see* Bellissent-Funel M.-C.

RICCI, M.A., *see* Andreani, C.
RICCI, M.A., *see* Benassi, P.
RICCI, M.A., *see* De Santis, A.
RICCI, M.A., RUOCCO, G., and SAMPOLI, M.: Raman spectra of water in the translational and librational regions. III. Temperature evolution by computer simulation with the TIP4P potential, **67**, 19
RICCI, S.M., *see* Tarjus, G.
RICHARDS, W.G., *see* Reynolds, C.A.
RICHARDSON, F.S., *see* Berry, M.T.
RICHARDSON, F.S., *see* Jayasankar, C.K.
RICHARDSON, F.S., *see* May, P.S.
RICHARDSON, F.S., *see* Tanner, P.A.
RICHARDSON, R.M., *see* Date, R.W.
RICHTER, H., *see* Knöckel, H.
RICHTER, K., *see* Morgner, H.
RICKAYZEN, G.: The structure of inhomogeneous molecular fluids: a restricted orientation model, **75**, 333
RICKAYZEN, G.: Phase transitions in molecular fluids. The restricted orientation model, **80**, 1093
RICKAYZEN, G., *see* Calleja, M.
RICKAYZEN, G., *see* Kalpaxis, P.
RICKAYZEN, G., *see* Moradi, M.
RICKAYZEN, G., *see* Powles, J.G.
RICKMAN, J.M., *see* Phillpot, S.R.
RIDLEY, T., *see* Lawley, K.
RIECKHOFF, K.E., *see* Chen, W.-H.
RIGBY, M.: Hard ellipsoids of revolution. Viral coefficients for prolate and oblate molecules, **66**, 1261
RIGBY, M.: Hard gaussian overlap fluids, **68**, 687
RIGBY, M.: Virial coefficients of hard convex molecules in two dimension, **78**, 21
RIGBY, M., *see* Ghazi, F.
RIGBY, M., *see* Goulding, C.W.
RIJKS, W., GERRITSEN, M., and WORMER, P.E.S.: Computation of the short range repulsion energy from correlated monomer wavefunctions in van der Waals dimers containing He, Ne and N_2, **66**, 929
RING, S.G., *see* Belton, P.S.
RIOS, M.A., *see* Vázquez, L.
RITTGER, E.: The chemical potential of liquid xenon by computer simulation, **69**, 853
RITTGER, E.: Can three-atom potentials be determined from thermodynamic data? **69**, 867
RITTGER, E.: An empirical three-atom potential for xenon, **71**, 79
RIRRGER, E.: Free energy of systems with several local minima by the acceptance ratio method, **79**, 1073
RIVAIL, J.-L., *see* Millot, C.
RIZZOLI, C., *see* Maniero, A.L.
ROBB, M.A., *see* Bernardi, F.
ROBERT, J.B., *see* Jalabert, D.
ROBERTO-NETO, O., *see* Ornellas, F.R.
ROBERTS, K.J., *see* Pavlides, P.
ROBINSON, G.W., *see* Zhu, S.-B.
ROBINSON, R.L., GWO, D.-H., and SAYKALLY, R.J.: Far infrared laser Stark spectroscopy of the Σ bending vibration of ArHCl. Strong evidence for a double minimum potential surface, **63**, 1201
ROBLEDO, A., *see* Romero-Rochin, V.
ROCCA, D., *see* De Santis, A.
ROCHE, A.L., *see* Huber, K.P.
ROCHE, A.L., *see* Gauyacq, D.
ROCHESTER, C.H., *see* Millar, G.J.
RÖDER, M., *see* Reh, M.

RODGER, A. GEDANKEN, A., and KLEIN, H.: Circular dichroism of molecules requiring two substituents for chirality, **72**, 803
RODGER, P.M.: Molecular dynamics with anisotropic site potentials: butane, **76**, 1385
RODGER, P.M., STONE, A.J., and TILDESLEY, D.J.: The intermolecular potential of chlorine. A three phase study, **63**, 173
RODRIGUES, S.V., MAITI, , A.K., REIS, H., and BAUMANN, W.: Electro optical emission measurements on a nonconjugated bichromophoric donor-acceptor molecule, **75**, 953
RODRIGUEZ, A.L., VEGA, C., FREIRE, J.J., and LAGO, S.: Improved results for the potential parameters of methyl and methylene obtained from second virial coefficients of n-alkanes, **80**, 1565
RODRIGUEZ-RUIZ, J.A., *see* Al-Derzi, A.R.
RODRIGUEZ-RUIZ, J., *see* Murrell, J.N.
ROEGGEN, I.: An analysis of hydrogen-bonded systems: $(HF)_2$, $(H_2O)_2$ and $H_2O...HF$, **70**, 353
ROEHRIG, M.A., and KUKOLICH, S.G.: Quadrupole coupling measurements on ClNO, **76**, 221
ROETTI, C., *see* Saunders, V.R.
ROETTI, C., *see* Silvi, B.
ROGERS, S.A., BRAZIER, C.R., BERNATH, P.F., and BRAULT, J.W.: Fourier transform emission spectroscopy of the $b^3\Pi_g$ - $a^3\Sigma_u^+$ transition of He_2, **63**, 901
ROGERS, S.A., *see* Douay, M.
ROMERO-ROCHIN, V., VAREA, C., and ROBLEDO, A.: Stress tensor of curved interfaces, **80**, 821
RONCERO, O., *see* Gianturco, F.A.
ROOS, B.O., *see* González-Luque, R.
ROOT, A., *see* Harris, R.K.
ROSCH, N., *see* Pyykkö, P.
ROSEN, M.E., *see* Gochin, M.
ROSINBERG, M.L., *see* Kierlik, E.
ROSLER, G., *see* Lang, A.
ROSMUS, P., *see* Brommer, M.
ROSMUS, P., *see* Carter, S.
ROSS, A.J., AMREIN, A., LUCKHAUS, D., and QUACK, M.: The rotational structure of the υ_4-band of $CH^{35}ClF_2$, **66**, 1273
ROSS, R.G., *see* Andersson, O.
ROSSI, V., *see* Ramondo, F.
ROSSLEIN, M., *see* Celii, F.G.
ROSSLEIN, M., *see* Hanratty, M.A.
ROSSLEIN, M., HANRATTY, M.A., and MAIER, J.P.: The r_s-structure of bromocyanogen cation: $BrCN^+$ $X^2\Pi$, **68**, 823
ROSSY-DELLUC, S., *see* Cartailler, T.
ROSTAS, J., *see* Le Floch, A.
ROTH, K., *see* Morgner, H.
ROUSSEAU, B., BOUTIN, A., FUCHS, A.H., and CRAVEN, C.J.: Melting of sulphur hexafluoride clusters by molecular dynamics simulation, **76**, 1079
ROWLANDS, T.W., *see* Bone, R.G.A.
ROWLEY, R.L., and ELY, J.F.: Non-equilibrium molecular dynamics simulations of structured molecules. Part 1. Isomeric effects on the viscosity of butanes, **72**, 831
ROWLEY, R.L., and ELY, J.F.: Non-equilibrium molecular dynamics simulations of structured molecules. II. Isomeric effects on the viscosity of models for *n*-hexane, cyclohexane and benzene, **75**, 713
ROWLINSON, J.S., *see* Baram, A.
ROWLINSON, J.S., and MCQUARRIE, D.A.: The third virial coefficient of hard discs of different sizes, **61**, 525
ROWLINSON, J.S., *see* Woods, G.B.
ROWLINSON, J.S., *see* Xiao, C.
ROYEN, P., *see* Berg, L.-E.
ROYEN, P., *see* Launila, O.

ROZANTSEV, E.G., OZHOGINA, O.A., RAKHIMOV, R.R., and PROKOF'EV, A.I.: The effect of molecular mobility on spin exchange on dinitroxylinacol, **76**, 1009
RUBAHN, H.-G., and SATHYAMURTHY, N.: Quasiclassical trajector study of Li_2 ($v < 25, j < 100$)-Na exchange reaction, **78**, 1047
RUCKER, S.P., *see* Gochin, M.
RUCKER, S.P., and SHAKA, A.J.: Broadband homonuclear cross polarization in 2D N.M.R. using DIPSI-2, **68**, 509
RUDISILL, E.N., and CUMMINGS, P.T.: Gibbs ensemble simulation of phase equilibrium in the hard core two-Yukawa fluid model for the Lennard-Jones fluid, **68**, 629
RUDOWICZ, C.: Correlations between orthorhombic crystal field parameters for rare-earty (F″) and transition-metal (d″) ions in crystals: $REBa_2Cu_3O_{7-x}$, $RE_2F_{14}B$, RE-garnets, RE: LaF_3 and MnF_2, **74**, 1159
RUIZ, M.E., *see* Jarque, C.
RULL, L.F., *see* De Miguel, E.
RULL, L.F., *see* Velarde, J.M.
RULLMANN, J.A.C., and VAN DUIJEN, P. TH.: Analysis of discrete and continuum dielectric models: application to the calculation of protonation energies in solution, **61**, 293
RULLMANN, J.A.C., and VAN DUIJEN, P. TH.: A polarizable water model for calculation of hydration energies, **63**, 451
RULLMANN, J.A.C., and VAN DUIJEN, P. TH.: A polarizable water model for calculation of hydration energies (erratum), **64**, 557
RUOCCO, G., *see* Benassi, P.
RUOCCO, G., *see* De Santis, A.
RUOCCO, G., *see* Gallo, P.
RUOCCO, G., *see* Maréchal, G.
RUOCCO, G., *see* Mazzacurati, V.
RUOCCO, G., *see* Ricci, M.A.
RUPPRECHT, A.: On the atomic polar tensor (APT) approach for vibrational circular dichroism (VCD) and Raman optical activity (ROA), **63**, 951
RUPPRECHT, A.: Sum rules for the rotational strength of fundamental transitions in vibrational circular dichroism (VCD), **63**, 955
RUSANOV, A.I., *see* Brodskaya, E.N.
RUSSELL, D.K., *see* Burie, J-R.
RUSSIER, V., and HENDERSON, D.: Size effect on the dielectric constant of the dipolar hard sphere fluid, **64**, 261
RUSSO, N., *see* Celebre, G.
RUSSO, N., *see* Sicilia, E.
RYCERZ, Z.A., and JACOBS, P.W.M.: Effective pair potentials in liquid metals. A comparative study for liquid lead, **74**, 425
RYCKAERT, J.-P., *see* Depaepe, J.M.
RYCKAERT, J.-P., *see* Dupont, G.
RYCKAERT, J.-P., *see* Maréchal, G.
RYCKAERT, J.-P., MCDONALD, I.R., and KLEIN, M.L.: Disorder in pseudohexagonal rotator phase of *n*-alkanes: molecular-dynamics calculations for tricosane, **67**, 957
RYCKAERT, J.-P., *see* Pierleoni, C.

SAAGER, B., *see* Fischer, J.
SAAGER, B., *see* Oelschlaeger, H.
SAAGER, B., *see* Vega, C.
SABEUR, Z.A., *see* Evans, R.
SABIN, J.R., *see* Geertsen, J.
SABOUNGI, M.-L., HOWE, M.A., and PRICE, D.L.: Structure and dynamics of molten aluminium and gallium trihalides. I. Neutron diffraction, **79**, 847
SACCHETTI, F., *see* Andreani, C.
SACCHETTI, F., *see* Montone, A.

SACCHETTI, F., *see* Petrillo, C.
SACHDEV, H.S., *see* Counsell, C.J.R.
SACHDEV, H.S., *see* Emsley, J.W.
SACHIKO NAKAI, YAMASHITA, A.B., and MEATH, W.J.: On neighbouring-level effects and the validity of the rotating-wave approximation, for a quasi-continuum five-level model doorway system, **71**, 1333
SADLEJ, A.J., *see* Fowler, P.W.
SADLEJ, A.J., *see* Kellö, V.
SADLEJ, A.J., *see* Lazzeretti, P.
SADLEJ, A.J., *see* Wolinski, K.
SADLER, I.A., *see* Kennedy, R.A.
SADLER, I.A., *see* Moss, R.E.
SADOVSKII, D.A., and ZHILINKSII, B.I.: Qualitative analysis of vibration-rotation hamiltonians for spherical top molecules, **65**, 109
SAENGER, W., *see* Steiner, Th.
SAEZ RABANOS, V., *see* Verdasco, E.
SAGDEEV, R.Z., *see* Valyaev, V.I.
SAINT-LOUP, R., *see* Lavorel, B.
SALASCO, L., DOVESI, R., ORLANDO, R., CAUSA, M., and SAUNDERS, V.R.: A periodic *ab initio* extended basis set study of *x*-Al_2O_3, **72**, 1135
SALASCO, L., *see* Saunders, V.R.
SALECK, A.H., WINNEWISSER, G., and YAMADA, K.M.T.: High resolution spectrum of $^{14}N^{16}O$ in the far infrared region: $^2\Pi_{3/2}$-$^2\Pi_{1/2}$ tranitions, **76**, 1443
SALECK, A.H., YAMADA, K.M.T., and WINNEWISSER, G.: Isotopic nitric oxide spectra and breakdown of the Born-Oppenheimer approximation, **72**, 1135
SALMON, A., *see* Brown, M.F.
SALTHOUSE, J.A., *see* Lindberg, P.
SALVETTI, O., *see* Fortunelli, A.
SALZMANN, S., *see* Wendland, M.
SAMBORSKI, A., and EVANS, G.T.: A phase diagram for non-spherical molecules with spherical square wells. Isotropic and nematic phases, **80**, 1257
SAMBORSKI, A., *see* Stecki, J.
SAMIOS, J., *see* Mittag, U.
SAMIOS, J., *see* Strehle, F.
SAMOSON, A., LIPPMAA, E., and PINES, A.: High resolution solid-state N.M.R. Averaging of second-order effects by means of a double-rotor, **65**, 1013
SAMPOLI, M., *see* Benassi, P.
SAMPOLI, M., *see* De Santis, A.
SAMPOLI, M., *see* Ricci, M.A.
SAMULSKI, E.T., *see* Photinos, D.J.
SANCHEZ-DE-MERAS, A.M., *see* Garcia-Guesta, I.
SANCTUARY, B.C., *see* Krishnan, M.S.
SÄNDIG, R., *see* Sonnenburg, J.
SANDLER, S.I., *see* Sowers, G.M.
SANE, R.N.: Monte Carlo simulation of a two-dimensional hexagonal monolayer of point dipoles, **71**, 509
SAN-FABIAN, J., *see* Diez, E.
SAN-FABIAN, J., *see* Esteban, A.L.
SAN-FABIAN, J., *see* Guilleme, J.
SANNA, N., *see* Gianturco, F.A.
SANTAMARIA, J., *see* Ayllón, A.G.
SANTIKARY, P., *see* Yashonath, S.
SANTOS, A., *see* Castaño, F.
SANTOS J., and ORZA, J.M.: Intensity parameters for the Raman trace and anisotropic scattering of methyl iodide, **70**, 645

SARICIFTCI, N.S., WERNER, A., and MEHRING, M.: Structural effects on the spin distribution anomaly of viologens, **75**, 1269
SARICIFTCI, N.S., WERNER, A., GRUPP, A., MEHRING, GÖTZ, G., BAUERLE, P., and EFFENBERGER, F.: On the spin distribution in bridged anthracene-viologen molecules: an electron-nuclear double resonance study, **75**, 1259
SARI-ZIZI, N.B., *see* Najib, H.
SARI-ZIZI, N.B., *see* Ouahman, M.
SARKA, K., and PAPOUSEK, D.: Determinable parameters of the effective rotational hamiltonians for excited vibrational states of semi-rigid symmetric top molecules, **65**, 829
SARMAN, S., *see* Evans, D.J.
SARMAN, S., *see* Kjellander, R.
SARRE, P.J., *see* Curtis, M.C.
SARRE, P.J., and WHITHAM, C.J.: New electronic transitions in the CH^+ molecule, **62**, 1505
SASSI, M.P., *see* Snels, M.
SASSI, P., and CATALIOTTI, R.S.: Intraband vibronic coupling between excited electronic states in *cis*-polyacetylene by Raman resonance scattering, **77**, 937
SASTRY, M.D., *see* Porwal, N.K.
SATHYAMURTHY, N., *see* Rubahn, H.-G.
SAUER, J., *see* Hill, J.-R.
SAUER, S.P.A., ODDERSHEDE, J., and GEERTSEN, J.: Correlated calculations of the rotational *g*-tensor and origin independent magnetizability surface of BH, **6**, 445
SAUNDERS, V.R., *see* Salasco, L.
SAUNDERS, V.R., FREYRIA-FAVA, C., DOVESI, L., SALASCO, L., and ROETTI, C.: On the electrostatic potential in crystalline systems where the charge density is expanded in Gaussian function, **77**, 629
SAUPE, A., *see* Chidichimo, G.
SAUVAGE, J.M., and DESCAMPS, M.: Influence of intermolecular correlations on the incoherent quasielastic neutron scattering, **65**, 1227
SAUVAJOL, J.L., *see* Guinet, Y.
SAVIN, A., *see* Ingel-Mann, G.
SAYKALLY, R.J. *see* Dz-Hung Gwo
SAYKALLY, R.J., *see* Elrod, M.J.
SAYKALLY, R.J., *see* Hovde, D.C.
SAYKALLY, R.J., *see* Hwang, H.J.
SAYKALLY, R.J., *see* Polak, M.
SAYKALLY, R.J., *see* Robinson, R.L.
SCAPPINI, F., *see* Caminati, W.
SCARABOTTO, P., *see* Maniero, A.L.
SCHAAF, P., *see* Talbot, J.
SCHAEFER, H.F., III, *see* Shen, M.
SCHAEFER, H.F., *see* Tozer, D.J.
SCHAEFER, H.F.,III, *see* Quelch, G.E.
SCHAEFER, H.F., III, *see* Xie, Yaoming
SCHAINK, H.M., *see* Wegdam, G.H.
SCHAMPS, J., *see* Le Floch, A.
SCHEFFLER, K., HOFLER, U., SCHULER, P., and STEGMANN, H.B.: Chiral recognition by formation of paramagnetic diasteromeric complexes, **65**, 439
SCHERAGA, H.A., *see* Gibson, K.D.
SCHERWINSKI, K.: Two approximations for the classical triplet distribution function, **70**, 797
SCHINDLER, H., VOGELSANG, R., STAEMMLER, V., SIDDIQI, M.A., and SVEJDA, P.: *Ab initio* intermolecular potentials of methane, nitrogen and methane + nitrogen and their use in Monte Carlo simulations of fluids and fluid mixtures, **80**, 1413
SCHLEGEL, H.G., *see* Gonzales, C.
SCHLIER, CH. G.: Angular momentum dependence of unimolecular decay in a triatomic system, **62**, 1009
SCHLIER, C., *see* Berblinger, M.

SCHLÖGL, R., *see* Atamny, F.
SCHMALTZ, T.G., *see* Poshusta, R.D.
SCHMIDT, A., *see* Frydman, L.
SCHMIDT, C., *see* Gochin, M.
SCHMIDT, K.E., *see* Tawa, G.J.
SCHMIDT-ROHR, K., *see* Zemke, K.
SCHMIDTKE, H.-H., *see* Degen, J.
SCHMIDTKE, H.-H., *see* Strand, D.
SCHMUTTENMAER, C.A., *see* Dz-Hung Gwo
SCHNEIDER, D., *see* Döge, G.
SCHNEIDER, F., ZULICKE, L., and CAHPUISAT, X.: A reaction-path description of the HO_2 reactive system, **71**, 17
SCHNEIDER, F., *see* Graf, H.-H.
SCHNEIDER, M., *see* Havenith, M.
SCHNITKER, J., *see* Naidoo, K.J.
SCHOEN, M., *see* Hertzner, A.W.
SCHOEN, M., RHYKERD, C.L., JR., CUSHMAN, J.H., and DIESTLER, D.J.: Slip-pore sorption isotherms by the grand-canonical Monte Carlo method. Manifestation of hysteresis, **66**, 1171
SCHOEN, M., DIESTLER, D.J., and CUSHMAN, J.H.: Isostress-isostrain ensemble Monte Carlo simulation of second order phase transitions in a confined monolayer fluid, **78**, 1097
SCHOFIELD, S.A., *see* Cina, J.A.
SCHOUTEN, J.A., *see* Kortbeek, P.J.
SCHOUTEN, J.A., *see* Sun, T.F.
SCHREIER, H.-J., *see* Karrlein, W.
SCHUG, J.C., *see* Gregory, V.P.
SCHULTE, J., *see* Böhm, M.C.
SCHULTE-HERBRUGGEN, T., MADI, Z.L, SORENSEN, O.W., and ERNST, R.R.: Reduction of multiplet complexity in COSY-type NMR spectra. The bilinear and planar COSY experiments, **72**, 847
SCHULER, P., *see* Scheffler, K.
SCHÜRMANN, B.L., *see* Depner, M.
SCHÜTT, J., *see* Böhm, M.C.
SCHROTTER, H.W., *see* Ouazzany, Y.
SCHWARZ, S.A.: Studies of surface and interface segregation in polymer blends by secondary ion mass spectrometer, **76**, 937
SCHWARTZ, M., *see* Wang, S.P.
SCHWARTZMANN, T., *see* Michelot, F.
SCHWEDA, H.S., *see* Norman, J.G.
SCHWERDTFEGER, P., *see* Dolg, M.
SCHWERDTFEGER, P., *see* Häussermann, U.
SCIORTINO, F., and CORONGIU, G.: Raman and infrared spectra of hexagonal ice between 0 and 400 cm^{-1}: a molecular dynamics simulation, **79**, 547
SCRIVEN, L.E., *see* Mier-y-Teran, L.
SCRIVEN, L.E., *see* Zixiang Tang
SCULLMAN, R., *see* Gustafsson, G.
SCUSERIA, G.E., *see* Colt, J.R.
SEAR, R.P., AMOS, M.D., and JACKSON, G.: Bonded hard-sphere theory and computer simulations of polyatomic hard-sphere models of alkanes and their derivatives, **80**, 777
SEARLES, D., *see* Eggenberger, R.
SEARS T.J., *see* Bogey, M.
SEARS, T.J., *see* Frye, J.M.
SEARS, T.J., *see* Northrup, F.J.
SEAVER, M., *see* Gauyacq, D.
SEDDON, J.M., *see* Date, R.W.
SEDDON, J.M., *see* Hamley, I.W.
SEDIAWAN, W.B., GUPTA, S., and MCLAUGHLIN, E.: Simulation and theory of fluids of axisymmetric molecules, **62**, 141

SEDIAWAN, W.B., GUPTA, S., and MCLAUGHLIN, E.: Simulation and theory of fluids of axisymmetric molecules. II. The modified gaussian overlap potential model, **63**, 691
SEDIAWAN, W.B., *see* Gupta, A.
SEEBASS, W., WERNER, J., URBAN, W., COMBEN, E.R., and BROWN, J.M.: The infrared spectrum of five isotopic forms of SiH radical by laser magnetic resonance, **62**, 161
SEEGER, S., *see* Botschwina, P.
SEGRE, U., *see* Burstolon, M.
SEGSCHNEIDER, C., *see* Härtl, W.
SEKI, H., *see* Yamada, T.
SEKINO, H., *see* Kobayashi, H.
SEMENOV, M.B., *see* Dakhnovskii, Yu. I.
SEMIONKIN, V.A., *see* Oshtrakh, M.I.
SEN, A.K., *see* Tjipto-Margo, B.
SENEKOWITSCH, J., *see* Carter, S.
SEPAROVIC, F., *see* Bowden, G.J.
SEPAROVIC, F., PAX, R., and CORNELL, B.: NMR order parameter analysis of a peptide plane aligned in a lyotropic liquid crystal, **78**, 357
SER, S., LARHER, Y., and BILQUIN, B.: Multilayer adsorption of xenon and argon on graphite. Wetting behaviour, **67**, 1077
SERNA, S., *see* Gianturco, F.A.
SESE, L.M.: Path-integral and effective potential Monte Carlo simulations of liquid nitrogen, hard-sphere and Lennard-Jones potentials, **74**, 177
SESE, L.M.: A quantum Monte Carlo study of liquid Lennard-Jones methane, path-integral and effective potentials, **76**, 1335
SESE, L.M.: Feynman-Hibbs quantum effective potentials for Monte Carlo simulations of liquid neon, **78**, 1167
SESE, G., *see* Padró, J.A.
SETHI, D.P.S., *see* Murad, S.
SETHI, D.P., *see* Powles, J.G.
SETHI, N.K., ALDERMAN, D.W., and GRANT, D.M.: NMR spectra from powdered solids spinning at any angle and speed; simulations and experiments, **71**, 217
SGARABOTTO, P., *see* Caciuffo, R.
SHAHAL, O., *see* Moreh, R.
SHAKA, A.J., *see* Cho, H.
SHAKA, A.J., *see* Mohebbi, A.
SHAKA, A.J., *see* Rucker, S.P.
SHALABI, A.S., KAMEL, M.A., SHALABI, S.A., and EID,KH. M.: Ground and excited state properties of many-body energies in $Li_n^{n+} + F^-$ ions, **75**, 1365
SHALABI, S.A., *see* Shalabi, A.S.
SHAOYI JIANG, RHYKERD, C.L., and GUBBINS, K.E.: Layering, freezing transitions, capillary condensation and diffusion of methane in slit carbon pores, **79**, 373
SHAOYI, JIANG, GUBBINS, K.E., and ZOLLWEG, J.A.: Absorption, isosteric heat and commensurate-incommensurate transition of methane on graphite, **80**, 103
SHAPTON, R.A., *see* Bucknall, R.E.
SHARMA, S.R.: Molecular association and the anisotropic-nematic transition, **78**, 733
SHELLEY, V., and YARWOOD, J.: Raman spectroscopic studies on the interaction and dynamics of N,N-dimethylformamide in the liquid phase. The effect of isotopic dilution, **72**, 1407
SHEN, D., and PRITCHARD, H.O.: Effect of rotation on molecular shape, **77**, 787
SHEN, D., and PRITCHARD, H.O.: Does black-body radiation cause intramolecular vibrational relaxation? **80**, 1135
SHEN, J.C., *see* Wang, C.H.
SHEN, M., and SCHAEFER, H.F., III: The fundamental vibrational frequencies of the silyl anion (SiH_3), **76**, 467
SHEN, M., SCHAEFER, H.F., III, and PARTRIDGE, H.: The remarkable enneahydridorhenate dianion: ReH_9^{2-}, **76**, 995
SHENYAVSKAYA, E.A., *see* Kaledin, L.A.

SHEOREY, V.B., *see* Sinha, S.
SHILSTONE, G.N., *see* Emsley, J.W.
SHING, K.S., GUBBINS, K.E., and LUCAS, K.: Henry constants in non-ideal fluid mixtures. Computer simulation and theory, **65**, 1235
SHINOHARA, T., *see* Sogami, I.S.
SHIOI, A., *see* Kinoshita, M.
SHIRAZI, A.R.B., and KNORR, K.: CF_2HCl monolayers physisorbed on graphite, **76**, 807
SHIRAZI, A.R.B., and KNORR, K.: Monolayers of C_2F_6 on graphite, **78**, 73
SHIRLEY, J.E., *see* Steimle, T.C.
SHKROB, I.A., *see* Batchelor, S.N.
SHUKLA, K.P.: Thermodynamic properties of simple fluid mixtures from perturbation theory, **62**, 1143
SHUKLA K.P., and HAILE, J.M.: Computer simulation results for thermodynamic excess properties in fluid mixtures. I. Effects of atomic size in simple mixtures, **62**, 617
SHUKLA, K.P., and HAILE, J.M.: Computer simulation results for thermodynamic excess properties in fluid mixtures. II. Effects of energy parameter differences in simple binary mixtures, **64**, 1041
SHUSIN, A.I.: Magnetic field effects in reactions of geminate recombination of anisotropic radicals, **64**, 65
SIBERT, E.L., III., *see* McCoy, A.B.
SICILIA, E., and RUSSUO, N.: Heat of formation of the hydroperoxyl radical (HO_2) determined using density functional theory, **76**, 1025
SIDDIQI, M.A., *see* Schindler, H.
SIDERS, P.: Monte Carlo study of a monolayer of hard oblate spheriods, **68**, 1001
SIEPMANN, J.I.: A method for the direct calculation of chemical potentials for dense chain systems, **70**, 1145
SIEPMANN, J.I., and FRENKEL, D.: Configurational bias Monte Carlo: a new sampling scheme for flexible chains, **75**, 59
SIEPMAN, J.I., *see* De Pablo, J.J.
SIEPMANN, J.I., and MCDONALD, I.R.: Monte Carlo simulations of mixed monolayers, **75**, 255
SIEPMANN, J.I., and MCDONALD, I.R.: Monte Carlo study of the properties of the self-assembled monolayers formed by adsorption of $CH_3(CH_2)_{15}SH$ on the (111) surface of gold, **79**, 457
SIESE, M., *see* Knöckel, H.
SILBERT, M., *see* Canessa, E.
SILBERT, M., *see* Gianotti, R.D.
SILBERT, M., *see* Gonzalez, D.J.
SILBERT, M., *see* Grimson, M.J.
SILBERT, M., *see* Jung Wang
SILLESCU, H., *see* Zemke, K.
SILVA, B., *see* Bouteiller, Y.
SILVA, B., *see* Le Duff, Y.
SILVI, B., CAUSA, M., DOVESI, R., and ROETTI, C.: Non-empirical pseudopotentials in the HF-LCAO approach to crystalline solids. Comparison to all-electron results, **67**, 891
SIMMONDS, P.S.J., *see* Luckhurst, G.R.
SIMMONS, R.O., *see* Herwig, K.W.
SIMON, U., *see* Huhn, B.
SIMON, U., *see* Lipus, K.
SIMON, U., *see* Petri, M.
SIMON, U., PETRI, M., ZIMMERMANN, W., and URBAN, W.: Infrared diode-laser spectroscopy of the ground state of SnH ($X\ ^2\Pi_{1/2}$), **71**, 1163
SIMON, U., PETRI, M., ZIMMERMANN, W., HUHN, G., and URBAN, W.: Infrared diode laser spectroscopy of the electronic ground state of SnD, **73**, 1051
SIMON, U., *see* Zimmermann, W.
SIMONIN, J.P., and MOREAU, M.: On the kinetics of diffusive liquids-liquid interfacial transport: mean-passage-time solution and the chemical picture, **70**, 265
SIMONS, J.P., *see* Brouard, M.

SIMONSON, T.: Free energy of particle insertion. An exact analysis of the origin singularity for simple liquids, **80**, 441
SIMPSON, N.J.K., *see* Valyaev, V.I.
SINGER, K., *see* Melrose, J.R.
SINGER, K., *see* Morales, J.J.
SINGER, K., and SMITH, W.: Path integral simulations of condensed phase Lennard-Jones systems, **64**, 1215
SINGH, A.K., and SINHA, S.K.: Equilibrium properties of molecular fluid mixtures in the semiclassical limit, **61**, 923
SINGH, D.P., *see* Murad, S.
SINGH, U.P., MOHANTY, U., and SINHA, S.K.: Perturbation theory of fluids of axisymmetric molecules. Gaussian overlap and modified gaussian overlap fluid models, **68**, 1047
SINGLETON, V.N., *see* Celebre, G.
SINHA, B., *see* Ramasesha, S.
SINHA, J.P., and SINHAL, S.K.: Semiclassical statistical mechanics of a ν-dimensional fluid of hard ν-spheres. Part II. Equilibrium properties of a dense hard ν-sphere fluid, **71**, 135
SINHA, S.K., *see* Dey, T.K.
SINHA, S.K., Semiclassical statistical mechanics of a ν-dimensional fluid of hard ν-spheres. I. Equilibrium properties of dilute hard ν-sphere gas, **69**, 587
SINHA, S., and RAMASWAMY, R.: Semiclassical quantization of resonant systems, **67**, 335
SINHA, S., and SHEOREY, V.B.: Discrete Hamiltonian symmetries and semiclassical quantization, **80**, 1525
SINHA, S.K., *see* Singh, A.K.
SINHA, S.K., *see* Sinha, J.P.
SIREGAR, J.J., *see* Mason, E.A.
SIRONI, M., COOPER, D.L., GERRATT, J., and RAIMONDI, M.: Spin-coupled VB study of the dications of methane, ammonia and water, **65**, 61
SIU, G.G., *see* Tanner, P.A.
SKELTON, N.J., *see* Palmer, A.G. III
SLAMAN, M.J., *see* Aziz, R.A.
SLANINA, Z., KURTZ, J., and ADAMOWICZ, L.: Is the C_8 ring nonplanar?, **76**, 387
SLEE, T., LE ROY, R.J., and CHUAQUI, C.E.: Calculated rovibratonal energy levels and infrared spectrum of He-C_2H_2, **77**, 111
SLOTH, P.: Electrochemical potentials in the grand canonical ensemble. Some formal and numerical results for confined ionic systems, **77**, 667
SLUCKIN, T.J., *see* Poniewierski, A.
SLUCKIN, T.J., *see* Teixeira, P.I.C.
SMALLEY, M.V.: Electrostatic interaction on macro-ionic solutions and gels, **71**, 1251
SMALLEY, M.V.: The ion distribution in *n*-butylammoniuim vermiculite gels, **76**, 1501
SMALLEY, M.V., and BALL, P.C.: The group theory of trigonal and tetrahedral molecule rotations in trigonal and tetrahedral crystal fields, **71**, 1233
SMALLEY, M.V., *see* Sogami, I.S.
SMENTEK-MIELCZAREK, L.: Electron correlation third-order contributions to the electric dipole transition amplitudes of rare earth ions in crystals. II. A general effective operator formulation based on static and dynamic models, **61**, 767
SMIT, B., COX, K.R., and MICHELS, J.P.J.: The influence of the quality of the solvent on the properties of a polymer. A thermodynamic model and molecular dynamics calculations, **66**, 97
SMIT, B., *see* de Leeuw, S.W.
SMIT, B., DE SMEDT, PH., and FRENKEL, D.: Computer simulations in the Gibbs ensemble, **68**, 931
SMIT, B., and FRENKEL, D.: Calculation of the chemical potential in the Gibbs ensemble, **68**, 951
SMIT, B., and FRENKEL, D.: Vapour-liquid equilibria of the hard core Yukawa fluid, **74**, 35
SMIT, B., *see* Frenkel, D.
SMIT, B., HAUSCHILD, T., and PRAUSNITZ, J.M.: Effect of a density-dependent potential on the phase behaviour of fluids, **77**, 1021
SMIT, B., *see* Mooij, G.C.A.M.
SMIT, B., *see* Van Leeuwen, M.E.

SMIT, B., WILLIAMS, C.P., HENDRIKS, E.M., and DE LEEUW, S.W.: Vapour-liquid equilibria for Stockmayer fluids, **68**, 765
SMITH, C.M., AMOS, R.D., and HANDY, N.C.: Theoretical calculations of the nuclear magnetic shielding tensors for the ethylenic carbon toms in cyclopropenes, **77**, 381
SMITH, D.J., *see* Firth, N.C.
SMITH, D.J., *see* Grice, R.
SMITH, D.J., and GRICE, R.: Angular distributions of reactive scattering arising from persistent complexes with asymmetric top transition states, **73**, 1371
SMITH, D.J., *see* Harkin, J.J.
SMITH, D.J., *see* Jarvis, R.D.
SMITH, E.B., *see* Evans, G.T.
SMITH, E.B., *see* Hunter, I.M.
SMITH, E.G., *see* Coveney, F.M.
SMITH, E.R.: Electrostatic potentials for simulations of thin layers, **65**, 1089
SMITH, E.R., and WIELOPOLSKI, P.A.: Dielectric constants from computer simulations. Periodic boundary conditions, sample size and behaviour of $\epsilon(k)$, **61**, 1063
SMITH, I.W.M., *see* Chewter, L.A.
SMITH, I.W.M., and YARWOOD, G.: A high resolution FTIR spectroscopic study of the hydrogen-bonded heterodimer H_3N-HCN, **64**, 627
SMITH, K.I., *see* Morris, G.A.
SMITH, S.W., *see* Emsley, J.W.
SMITH, W., *see* Singer, K.
SMITH, W.R., and LABIK, S.: Two new exact criteria for hard-sphere mixtures, **80**, 1561
SMITH, W.R., *see* Labik, S.
SMITH, W.R., *see* Malijevský, A.
SMITH, W.R., *see* Nezbeda, I.
SMITH, W.R., *see* Pospíšil, R.
SMITS, G.F., KROL, M.C., and ALTONA, C.: Theoretical investigations of the nature of intramolecular interactions. II. Application of the energy decomposition scheme to CH_3NH_2. CH_3OH, NH_2OH and HOOH, **63**, 921
SMITS, G.F., KROL, M.C.,and ALTONA, C.: Theoretical investigations on the nature of intramolecular interactions. III. Application of the energy decomposition scheme to the study of the anomeric effect in CH_3CCH_2OH, NH_2CH_2OH, $HOCH_2OH$ and FCH_2OH, **65**, 513
SMOLKA, K.-P., *see* Zimmermann, W.
SNAAR, J.E.M., *see* Hills, B.P.
SNELS, M., *see* Fantoni, R.
SNELS, M., *see* Hollenstein, H.
SNELS, M., *see* Nencini, L.
SNELS, M., SASSI, M.P., and QUACK, M.: High-resolution Fourier-transform infrared spectroscopy of the $\upsilon_3(F_2)$ fundamental of RuO_4, **72**, 145
SODERMAN, O., *see* Brown, M.F.
SOFTLEY, T.P., *see* Merkt, F.
SOGAMI, I.S., SHINOHARA, T., and SMALLEY, M.V.: Effective interaction of highly charged plates in an electrolyte, **74**, 599
SOGAMI, I.S., SHINOHARA, T., and SMALLEY, M.V.: Adiabatic pair potential of highly charged plates in an electrolyte, **76**, 1
SOKOLOWSKI, S.: Adsorption of oxygen in slit-like pores: grand canonical ensemble Monte Carlo studies, **75**, 999
SOKOLOWSKI, S.: Molecular dynamics studies of adsorption and flow of fluids through geometrically non-uniform cylindrical pores, **75**, 1301
SOKOLOWSKI, S., and FISCHER, J.: Density functional theory for inhomogeneous fluids. Effects of triple correlations, **68**, 647
SOKOLOWSKI, S., and FISCHER, J.: Classical multicomponent fluid structure near solid substrates: Born-Green-Yvon equation versus density-functional theory, **70**, 1097
SOKOLOWSKI, S., and FISCHER, J.: Lennard-Jones mixtures in slit-like pores: a comparison of simulation and density-functional theory, **71**, 393

SOKOLOWSKI, S., *see* Patrykiejew, A.
SOLANA, J.R., *see* Maeso, M.J.
SOLONENKO, A.O., *see* Bersuker, G.I.
SOLUM, M.S., FACELLI, J.C., GAN, Z., and GRANT, D.M.: ^{13}C Dipolar spectroscopy of nitromethane, **64**, 1031
SOMOZA, A.M., and TARAZONA, P.: Density functional theory of the elastic constants of a nematic liquid crystal, **72**, 911
SOMOZA, A.M., and TARAZONA, P.: Liquid crystals of asymmetric hard body molecules, **75**, 17
SONG, Y., *see* Ihm, G.
SONNENBURG, J., KREMP, D., and SÄNDIG, R.: On the density dependence of the self-diffusion coefficient of interacting Brownian particles, **72**, 873
SONNENBURG., J., KREMP, D., and SÄNDIG, R.: Diffusion processes in Brownian particle systems with short-range interaction, **74**, 649
SOOD, A.K., *see* Tata, B.V.R.
SOON-CHUL KIM, JAE-KWAN SUH and SOONG-HYUCK SUH: Density profiles of fluids confined in a spherical cavity, **79**, 1369
SOONG-HYUCK SUH, *see* Soon-Chul Kim
SOPER, A.K., *see* Andreani, C.
SOPER, A.K., *see* Turner, J.
SOPER, A.K., TURNER, J., and FINNEY, J.L.: Solute-solute correlations in aqueous solutions of tetramethylammonium chlorine, **77**, 431
SORCE, D.J., KATZ, J., and CZEGLEDY, F.P.: Multiple-quantum filters of arbitrary phases for spin 3/2 nuclei, **80**, 1067
SORENSEN, O.W.,*see* Griesinger, C.
SORENSEN, O.W., *see* Schulte-Herbreggen, T.
SOUMPASIS, D.M., *see* Hummer, G.
SOURISSEAU, C., *see* Guillaume, F.
SOUSSEN-JACOB, J., GOULAY, A.M., and COHEN DE LARA, E.: Effect of an electric field on a methane molecule. I. Infrared analysis of methane adsorbed in CaA zeoline, **76**, 1037
SOUSSEN-JACOB, J., *see* Cohen de Lara, E.
SOWERS, G.M., and SANDLER, S.I.: Simulation results and corresponding states correlation for pure rigid molecular fluids, **77**, 35!
SPEEDY, R.J.: Diffusion in the hard sphere fluid, **62**, 509
SPEEDY, R.J.: The entropy of a glass, **80**, 1105
SPEEDY, R.J., and REISS, H.: A computer simulation study of cavities in the hard disc fluid and crystal, **72**, 1015
SPEEDY, R.J., and REISS, H.: Cavities in the hard sphere fluid and crystal and the equation of state, **72**, 9999
SPEEDY, R.J., PRIELMEIER, F.X., VARDAG, T., LANG, E.W., and LUDEMANN, H.-D.: Diffusion in simple fluids, **66**, 577
SPIESS, H.W., *see* Dahm, J.
SPIESS, H.W., *see* Günther, E.
SPIESS, H.W., *see* Zemke, K.
SPINDLER, T., *see* Karrlein, W.
SPIRKO, V., *see* Hettner, W.
SPOHR, E., *see* Trokhymchuk, A.D.
SPOOREN, R., *see* de Haag, P.U.,
SREEHARI, N., and MANOHARAN, P.T.: Triplet-state E.P.R. studies of exchange coupled copper (II) and silver (II) pairs in zinc (II) bis[N,N-diisopropyldithiocarbamate], **63**, 1077
SRIVASTAVA, S., and VISHWAMITTAR : Energies of oscillators with mixed quartic and sextic anharmonicities, **72**, 1285
STACE, A.J., *see* Marks, A.J.
STACE, A.J., OHASHI, K., LABLANQUIE, P., and NISHI, N.: Chemical reactivity promoted by optical excitation transfer in mixed clusters, **75**, 741
STACKMANN, V., LIPUS, K., and URBAN, W.: The infrared laser magnetic resonance spectrum of SbH ($X^1\Sigma^-$) nuclei, **80**, 635

STAEMMLER, V., *see* Schindler, H.
STAIKOVA, M., ENGELS, B., PERIC, M., and PEYERIMHOFF, S.D.: *Ab initio* calculations of the vibronically averaged hyperfine coupling constants in the $1^2\Pi_u(X^2B_1, A^2A_1)$ state of the water cation, **80**, 1485
STAPLETON, M., *see* Panagiotopoulos, A.Z.
STARIKOV, E.B.: On the convergence of the Hartree-Fock selfconsistency procedure, **78**, 285
STARIKOV, E.B.: On the electronic subsystem of nucleic acid crystallohydrages. Do nucleotides remain intact in the solid state?, **80**, 1459
STECKI, J., SAMBORSKI, A., and TOXVAERDS, S.: Henry constant of large solutes by simulation, **79**, 985
STEELE, W.A.: A theoretical approach to the calculation of time-correlation functions of several variables, **61**, 1031
STEELE, W.A.: Detailed balance factors for freely rotating linear molecules, **76**, 1265
STEELE, W.A., *see* Bhethanabotla, V.R.
STEELE, W.A., *see* Toro-Labbé, A.
STEELE, W.A., *see* Lustig, R.
STEELE, W.A., and VALLAURI, R.: Computer simulations of pair dynamics in molecular fluids, **61**, 1019
STEGEMANN, H., *see* Bengtsson, L.A.
STEGEMANN, H.B., *see* Scheffler, K.
STEIBEL, J., *see* Grucker, D.
STEIMLE, T., NACHMAN, D.F., SHIRLEY, J.E., FLETCHER, D.A., and BROWN, J.M.: The microwave spectrum of NiH, **69**, 923
STEINER, E., *see* Fowler, P.W.
STEINER, TH., SAENGER, W., and LECHNER, R.E.: Dynamics of orientationally disordered hydrogen bonds and of water molecules in a molecular cage. A quasielastic neutron scattering study of β-cyuclodextrin - $11H_2O$, **72**, 1211
STEINER, U.E., *see* Hamilton, C.A.
STEINER, U.E., *see* McLauchlan, K.A.
STELL, G., *see* Høye, J.S.
STELL, G., *see* Kalyuzhnyi, Yu, V.
STELL, G., *see* Lee, S.H.
STELL, G., *see* Zhou, Y.
STERNBERG, U.: Theory of the influence of the second co-ordination sphere on the chemical shift, **63**, 249
STERNBERG, U., *see* Hallas, E.
STETTER, M., MAULWURF, M., and MULLER, A.: Dynamics of methyl groups in pyrimidine 5-yl radicals studied by ENDOR spectroscopy, **72**, 607
STEYERT, D.W., *see* Elrod, M.J.
STICKLAND, R.J., *see* Allen, J.M.
STICKLAND, R.J., *see* Ashfold, M.N.R.
STILBS, P., *see* Laaksonen, A.
STOLL, H., *see* Bergner, A.
STOLL, H., *see* Dolg, M.
STOLL, H., *see* Häussermann, U.
STOLL, H., *see* Igel-Mann, G.
STOLL, H., *see* Küchle, W.
STONE, A.J., *see* Bone, R.G.A.
STONE, A.J, *see* Le Sueur, C.R.
STONE, A.J., *see* McDowell, S.A.
STONE, A.J., *see* Millot, C.
STONE, A.J., *see* Rodger, P.M.
STONE, A.J., and WALES, D.J.: A new structural tensor surface harmonic bonding theory, **61**, 747
STRAND, D., LINDER, R., and SCHMIDTKE, H.-H.: The vibronic structure of mixed-ligand osmium (IV) complexes. Part I. Low-energy levels of $OsCl_5X^{2-}$ and *cis*-$OsCl_4X_2^{2-}$ (X = Br,I), **71**, 1075
STRANGE, J.H., *see* Coveney, F.M.

STRANGER, R., MORAN, G., KRAUSZ, E., GUDEL, H., and FURER, N.: Octahedral monomeric molybdenum(III). A magneto-optical study of Mo^{3+} doped in Cs_2NaYCl_6, **69**, 11
STRATY, G.C., *see* Hanley, H.J.M.
STRATY, G.C., PIEPER, J., and HANLEY, H.J.M.: Contrast matched studies of a sheared binary colloidal suspension, **72**, 241
STRAUB, J.E.: Analysis of the role of attractive forces in self-diffusion of a simple fluid, **76**, 373
STRAUSS, M., *see* Peng, W.-G.
STRAVER, L., *see* André, D.
STREHLE, F., DORFMÜLLER, TH., and SAMIOS, J.: Concentration effects on collision-induced depolarized Rayleigh lineshapes in Cs_2/CCl_4 mixtures, **72**, 993
STREHLE, F., and DORFMÜLLER, TH.: Concentration effects on absolute depolarized Rayleigh ratios and effective polarizability derivatives of CS_2 in liquid mixtures with CCl_4, **77**, 339
STREHLE, F., and DORFMÜLLER, TH.: Raman spectroscopic study of the single dynamics of CS_2 in liquid binary mixtures with CCl_4, **80**, 449
STRINGAT, R., *see* Bernard, A.
STRYCZEK, B., and BRODKA, A.: A study of the influence of Fermi resonance on the Raman spectra of liquid ammonia, **62**, 365
STRYCZEK, B., *see* Brödka, A.
STYRKAS, D.A., *see* Li, Z.X.
SU, M.-D., *see* Pinnavaia, N.
SU, MING-DER: Relative strengths of axial and equatorial bonds and site preferences for ligand substitution in σ-bonded T-shaped EL_3 complexes, **80**, 1223
SU, M-D., WILLETTS, A., BRAMLEY, M.J., and HANDY, N.C.: A study of the ground electronic state of disulphane, **73**, 1209
SUBTIL, J.L., *see* Perrot, J.P.
SUENRAM, R.D., *see* Karyakin, E.N.
SUHM, M.A., *see* Quack, M.
SUHM, M.A., *see* von Puttkamer, K.
SUHM, M.A., and WATTS, R.O.: Parameterized dipole moment function for the water molecule, **73**, 463
SULLIVAN, D.E., *see* Joslin, C.G.
SULLIVAN, D.E., *see* Tjipto-Margo, B.
SULLIVAN, D.E., *see* Yang, B.
SUN, T.F., and SCHOUTEN, J.A.: The importance of accurate numerical integration in perturbation theories of molecular liquids, **69**, 601
SUN, T.F., and SCHOUTEN, J.A., TEN SELDAM, C.A., and BISWAS, S.N.: Perturbation calculation of thermodynamic properties of liquid benzene using the six centre Lennard-Jones potential, **69**, 615
SUN, T.F., SCHOUTEN, J.A., TEN SELDAM, C.A., and KORTBEEK, P.J.: An efficient algorithm for the solution of the correlation function for soft spherical repulsions, **69**, 607
SUTCLIFFE, B.T.: The use of perimetric coordinates in the vibration-rotation Hamiltonian for triatomic molecules, **75**, 1233
SUTCLIFFE, B.T., *see* Burden, F.R.
SUTCLIFFE, B.T., *see* Le Sueur, C.R.
SUTCLIFFE, B.T., *see* Miller, S.
SUTER, D., CHINGAS, G.C., HARRIS, R.A., and PINES, A.: Berry's phase in magnetic resonance, **61**, 1327
SUTER, D., *see* De Pablo, J.J.
SUTER, D., ERNST, M., and ERNST, R.R.: Quantum time-translation machine. An experimental realization, **78**, 95
SUZUKI, Y., OKAZAKI, S., and OKADA, I.: Isotope and temperature effects of the vibrational and rotational relaxation in molten alkali hydroxides, **76**, 1131
SVEIJDA, P., *see* Schindler, H.
SVENSSON, BO R., and WOODWARD, C.E.: Widom's method for uniform and non-uniform electrolyte solutions, **64**, 247
SWAMY, K.N., *see* Rami Reddy, M.

SYMONS, M.C.R., *see* Ferrario, M.
SÝS, J., *see* Pospíšil, R.
SZABO, A., *see* Pastor, R.W.
SZALAY, V., and LANE, S.: Derivation of rotational-vibrational Hamiltonian matrices of real elements, **75**, 781
SZAMEL, G., and PIASECKI, J.: Depolarized interaction-induced light scattering: a kinetic-theory approach, **70**, 783
SZCZESNIAK, M.M., *see* Chalasiński, G.
SZCZESNIAK, E., *see* Andrew, E.R.
SZLEIFER, I., and WIDOM, B.: Surface tension, line tension, and wetting, **75**, 925
SZLEIFER, I., *see* Perkovic, S.
SZWARC, H., *see* André, D.

TABISZ, G.C., *see* El-Sheikh, S.M.
TAE-KYU, HU, *see* Minh Tho Nguyen
TAJIMA, Y., *see* Morishige, K.
TAKACS, S.F., *see* Hills, B.P.
TAKAGI, R., *see* Adya, A.K.
TAKAGI, R., *see* Naito, S.
TAKAMI, M., *see* Matsumoto, Y.
TAKAMI, M., and MATSUMOTO, Y.: Free jet infrared absorption spectroscopy of the υ_3 band of MOF_6, **64**, 645
TAKAMIYA,M., and NAKANISHI, K.: Density-functional approach to two-dimensional classical fluids, **70**, 767
TAKEKIYO, S.: *Ab initio* calculations of the π-electron structures of aniline by the valence-bond method, **63**, 407
TALBOT, J.: A statistical model for the dynamical properties of hard body fluids, **75**, 43
TALBOT, J., PERERA, A., and PATEY, G.N.: A comparison between molecular-dynamics and theoretical results for the structure of fluids of hard ellipsoids, **70**, 285
TALBOT, J., SCHAAF, P., and TARJUS, G.: Random sequential addition of hard spheres, **72**, 1397
TALBOT, J., *see* Tarjus, G.
TALUKDAR, R., BAJAJ, P.N., CHAKRABORTI, P.K., and KARTHA, V.B.: Condensation of SF_6 in seeded supersonic jets, **80**, 127
TAN, K.L. *see* Kang, E.T.
TAN, Z., VAN SWOL, F., and GUBBINS, K.E.: Lennard-Jones mixtures in cylindrical pores, **62**, 1213
TANAKA, H., WALSCH, J., and GUBBINS, K.E.: Structure of water-methanol binary mixtures: role of the water-water interactions, **76**, 1221
TANAKA, K., *see* Hwang, H.J.
TANAKA, K., *see* Morita, T.
TANG, S., and EVANS, G.T.: A critique of slip and stick hydrodynamics for ellipsoidal bodies, **80**, 1443
TANG, Z., *see* Mier-y-Teran, L.
TANI, A., *see* Bertolini, D.
TANNER, P.A.: Luminescence and radiative decay of Er^{3+} in $CS_2NaErCl_6$, **63**, 365
TANNER, P.A., JAYASANKAR, C.K., and RICHARDSON, F.S.: Electronic spectra and crystal-field analysis of $DyCl_6^+$ in elpasolite lattices, **65**, 49
TANNER, P.A., *see* Flint, C.D.
TANNER, P.A., *see* Jayasankar, C.K.
TANNER, P.A., and SUI, G.G.: Electric quadrupole allowed transitions of lanthanide ions in octahedral symmetry, **75**, 233
TARAN, J.P., *see* Attal-Trétout, B.
TARAZONA, P.: A density functional theory of melting (erratum), **61**, 789
TARAZONA, P., *see* Navascués, G.
TARAZONA, P., *see* Somoza, A.M.
TARAZONA, P., *see* Telo da Gama, M.M.

TARJUS, G., *see* Dayan, E.
TARJUS, G., *see* Talbot, J.
TARJUS, G., VIOT, P., RICCI, S.M., and TALBOT, J.: New analytical and numerical results on virial coefficients for 2-D hard convex bodies, **73**, 773
TARRONI, R., *see* Arcioni, A.
TARRONI, R., *see* Bearpark, M.J.
TASSET, F., *see* Day, P.
TATA, B.V.R., KESAVAMOORTHY, R., and SOOD, A.K.: Structure factor for a two component mixture of dilute colloidal suspensions, **61**, 943
TAU, M., *see* Meroni, A.
TAWA, G.J. WHITLOCK, P., SCHMIDT, K.E., and MOSKOWITZ, J.W.: Monte Carlo calculation of interaction energies for van der Waals complexes, **77**, 477
TAYLOR, A.D., *see* Andreani, C.
TEFFO, J.L.: Born-Oppenheimer effects and vibration-rotational spectra of linear molecules. I. Theory, **78**, 1493
TEFFO, J.-L., and OGILVIE, J.F.: Born-Oppenheimer effects and vibration-rotational spectra of linear molecules. II. Application to CO_2, **80**, 1507
TEIXEIRA, P.I.C., PERGAMENSHCHIK, V.M. and SLUCKIN, T.J.: A model calculation of the surface elastic constants of a nematic liquid crystal, **80**, 1339
TEJERO, C.F., *see* Ferrero, F.S.
TEKELY, P.: Inhomogeneous distribution of correlation times in two-side exchange of phenyl groups and premelting of 4-ethoxyphenyl 4-ethoxybenzoate as revealed by high-resolution ^{13}C and ^{1}H solid-state NMR spectroscopy, **75**, 747
TEKELY, P., CANET, D., and DELPUECH, J.-J.: Observation of $^{1}Ä$ nuclei in heterogeneous solids via cross-polarization ^{13}C N.M.R., **67**, 81
TEKELY, P., *see* Jalabert, D.
TELEMAN, O., *see* Wallqvist, A.
TELEMAN, O., *see* Westlund, P.-O.
TELLINGHUISEN, J., *see* Lawley, K.P.
TELFER, J.M., *see* Inaba, A.
TELO DA GAMA, M.M.: Phase equilibria and interfacial properties of model ternary mixtures, **62**, 585
TELO DA GAMA, M.M., TARAZONA, P., ALLEN, M.P., and EVANS, R.: The effect of confinement on the isotropic-nematic transition, **71**, 801
TEMME, F.P.: Symmetry-adapted bases over Liouville space. V.$[A]_4$ ($I_i \geq 1$) related spin systems: Generation of the $|IM\alpha.\mu(S_4)>$ and $|kqv.\mu(S_4)>$ sets from the combinatorics of weight sets (M_4 - M_4), **66**, 1075
TEMME, F.P.: Structure of higher unitary dualities revisited. A model 'Met-^{13}Carb' NMR spin cluster problem, **78**. 747
TEMME, F.P., and COPLA, J.P.: Aspects of J pathways in $[A]_n(S_0)/[AX]$ spin systems over partitional, or coherent superpositional, Liouville space bases involving intracluster coupling, or associated with coherence transfer in [A...X], I_i = ½) systems: further group theoretical considerations, **73**, 953
TEMME, F.P., MITCHELL, C.E.J., and KRISHNAN, M.S.: Distinctive combinatorial aspects of NMR spin invariance for icosahedral exo-cage spin cluster problems: symmetry subduction and [λ] (S_{60}, $p \leq 3,4$) → $\Gamma(S_{60}{}^{\downarrow}\Im)$ mapping for ^{13}C-fullerene and the analogous biclusters systems, $[^{13}C]^{6}_{60}$, $[^{12}CF]_{60}$, and $[^{13}CF]_{60}$, **79**, 953
TEMME, F.P., *see* Kriskhan, M.S.
TEN SELDAM, C.A., *see* Kortbeek, P.J.
TEN SELDAM, C.A., *see* Sun, T.F.
TENNYSON, J., *see* Ayllon, A.G.
TENNYSON, J., *see* Henderson, J.R.
TENNYSON, J., *see* Le Sueur, C.R.
TENNYSON, J., *see* Miller, S.
TERAO, T., *see* Nakai, T.
TER BEEK, L.C., ZIMMERMAN, D.S., and BURNELL, E.E.: The conformation of 2,2′-dithiophene in nematic solvents determined by ^{1}H-NMR, **74**, 1027

TER BEEK, C., ZIMMERMANN, S., and BURNELL, E.E.: The orientation of molecules with internal rotation in nematic phases, **80**, 177
TERZIS, A.F., *see* Photinos, D.J.
TFIRST, E., *see* Kozmutza, C.
THAKKAR, A.J., *see* Hettema, H.
THAKKAR, A.J., *see* Komasa, J.
THAKKAR, A.J., *see* Maroulis, G.
THAMARAICHELVAN, A., *see* Murugesan, R.
THAMM, R., *see* Krienke, H.
THAYER, A.M., *see* Luzar, M.
THEODORAKOPOULOS G., PETSALAKIS, I.D., and BUENKER, R.J.: Theoretical calculations of the Rydberg spectra of ArH, **71**, 1055
THEODORAKOPOULOS, G., *see* Petsalakis, I.D.
THEODOROU, D.N., *see* Dodd, L.R.
THEWALT, M.L.W., *see* Chen, W.-H.
THIBEAU, M., *see* Barreau, A.
THIEL, W.: Nonlinear transformation of anharmonic normal coordinate force constants, **68**, 427
THOMAS, R.K., *see* Bucknall, R.E.
THOMAS, R.K., *see* Clarke, S.M.
THOMAS, R.K., *see* Inaba, A.
THOMAS, R.K., *see* Joshi, Y.P.
THOMAS, R.K., *see* Li, Z.X.
THOMAS, R.K., *see* Morishige, K.
THOMAS, R.K., *see* Penfold, J.
THOMPSON, S.M., *see* Cooney, W.R.
TIEMANN, E.: On the spectroscopic determination of potential functions with a barrier for diatomic molecules, **65**, 359
TIEMANN, E., *see* Bovensmann, H.
TIEMANN, E., *see* Knöckel, H.
TIEMANN, E., *see* Kröckertskothen, T.
TILDESLEY, D.J., *see* Joshi, Y.P.
TILDESLEY, D.J., *see* Hammonds, K.D.
TILDESLEY, D.J., *see* Leggetter, S.
TILDESLEY, D.J., *see* Panagiotopoulos, A.Z.
TILDESLEY, D.J., *see* Rodger, P.M.
TILDESLEY, D.J., Professor John S. Rowlinson, **80**, 701
TIMPE, O., *see* Atamny, F.
TINTI, D.S., *see* Neugebauer, S.M.
TISSEN, J.T.W.M, and JANSSEN, G.J.M.: Molecular-dynamics simulation of molten alkali carbonates, **71**, 413
TJIPTO-MARGO, B., and EVANS, G.T.: A van der Waals theory of nematic liquid crystals: a 'convex peg in a round hole' potential, **74**, 85
TJIPTO-MARGO, B., SENB, A.K., MEDEROS, L., and SULLIVAN, D.E.: The liquid-vapour interface of nematic liquid crystals, **67**, 601
TJIPTO-MARGO, B., *see* Yang, B.
TÖDHEIDE, K., *see* Bausenwein, T.
TOJO, C., *see* López-Quintela, M.A.
TOLE, P., *see* Fowler, P.W.
TOLONEN, A.-M., and ALANKO, S.: Investigation on the infrared spectrum of acetylene between 2500 cm^{-1} and 2800 cm^{-1} and studies of the resonance effects, **75**, 1155
TOMASELLO, P., and VON NIESSEN, W.: Electronic structure of lithium halide monomers and dimers : ionization energies and electron affinities, **69**, 1043
TOMSAH, I.B.I., *see* Clough, S.
TONGE, K.H., *see* Duncan, J.L.
TORCHET, G., *se* Bénière, F.M.
TORIUMI, H., *see* Photinos, D.J.

TORO-LABBE, A., LUSTIG, R., and STEELE, W.A.: Specific heats for simple molecular fluids from molecular dynamics simulations, **67**, 1385
TORRIE, B.H., BINBREK, O.S., and VON DREELE, R.: Crystal structure of chloroiodomethane, **79**, 869
TORRIE, B.H., *see* Ikram, A.
TORRIE, B.H., and POWELL, B.M.: Phase transition in solid acetonitrile, **75**, 613
TORRIE, B.H., *see* Prystupa, D.A.
TORRIE, B.H., VON DREELE, R., and LARSON, A.C.: Structure of solid cyanamide at 13K, **76**, 405
TORRIE, B.H., *see* Weng, S.-X.
TORRIE, G.M., PERERA, A., and PATEY, G.N.: Reference hypernetted-chain theory for dipolar hard spheres at charged surfaces, **67**, 1337
TORRIE, G.M., WENG, S.-X., and POWELL, B.M.: Structure of the α-phase of solid methanol, **67**, 575
TORII, Y., *see* Kobayashi, H.
TORRING, T., and HERRMANN, R.: Fine and hyperfine structure in the $X^2\Sigma^+$-state of AlO, **68**, 1379
TOSI, M.P. *see* Badirkham, Z.
TOSSELL, J.A., *see* McMillan, K.
TOWLE, J.P., and BROWN, J.M.: The infrared spectrum of the GeH radical by laser magnetic resonance, **70**, 161
TOWLE, J.P., and BROWN, J.M.: The infrared spectrum of the TeD radical by laser magnetic resonance, **74**, 465
TOWLE, J.P., and BROWN, J.M.: The infrared spectrum of the GeH radical, **78**, 249
TOWLE, J.P., BROWN, J.M., LIPUS, K., BACHEM, E., and URBAN, W: The infrared spectrum of the FeH radical by magnetic resonance, **79**, 835
TOWLE, J.P., *see* Petri, M.
TOXVAERD, S.: Algorithms for canonical molecular dynamics simulations, **72**, 159
TOXVAERD, S.: Distribution functions in liquid mixtures: molecular dynamics simulations and mean field theory, **76**, 1397
TOXVAERD, S., *see* Padilla, P.
TOXVAERD, S., *see* Stecki, J.
TOZER, D.J., HANDY, N.C., AMOS, R.D., POPE, J.A., NOBES, R.H., YAOMING, XIE and SCHAEFER, H.F.: Theory and application of spin-restricted open-shell Møller-Plesset theory, **79**, 777
TRELOAR, R.L., and MASTERS, A.J.: Short-time rotational diffusion of spheres in suspension, **67**, 1273
TRELOAR, R.L., ands MASTERS, A.J.: Short-time diffusion of anisotropic particles in suspension - a perturbative approach, **74**, 1195
TRENTINI, F.W., VOITLÄNDER, J., and BRÄUCHLE, C.: Resonance theoretical description of magnetic zero field splitting energies of benzenoid hydrocarbons. Structural dependence of the parameter *D*, **74**, 553
TRIBOLLET, B., *see* Broyer, M.
TRISC, M., *see* da Costa, H.F.M.
TRISC, M., *see* da Silva, A.B.F.
TŘÍSKA, B., and BOUBLÍK, T.: The chemical potential of non-spherical solute in the infinitely diluted mixture, **76**, 113
TROKHYMCHUK, A.D., HOLOVKO, M.F., SPOHR, E., and HEINZINGER, K.: Combination of computer simulation methods and optimized cluster theory in determining equilibrium properties of electrolyte solutions. I. General expressions and applications to pure water, **77**, 903
TROKHYMCHUK, A.D., HOLOVKO, M.F., and HENDERSON, D.J.: The contribution of dipole alignment to the force between macroions in an ion-dipole fluid, **80**, 1009
TRULLAS, J., *see* Padró, J.A.
TRUSLER, J.P.M.: On the inversion of thermophysical properties, **64**, 1153
TSUKERBLAT, B.S., PALII, A.V., KISHINEVSKY, H.M. GAMURAR,, V. YU and BERENGOL'TS, A.S.: Magnetic moments of the dimeric multielectronic mixed valence clusters in the dynamic model of intermediate vibronic coupling, **76**, 1103
TSUKERBLAT, B.S., *see* Gatteschi, D.
TUCKETT, R.P., *see* Creasey, J.C.
TUCKETT, R.P., *see* Mason, S.M.

TURQ, P., *see* Cartailler, T.
TURNER, J., SOPER, A.K., and FINNEY, J.L.: A neutron-diffraction study of tetra-methylammonium chloride in aqueous solution, **70**, 679
TURNER, J., SOPER, A.K. and FINNEY, J.L.: Water structure in aqueous solutions of tetramethylammonium chloride, **77**, 411
TURNER, J., *see* Soper, A.K.
TURNER R., *see* Cory, D.G.
TURULSKI, J., and NIEDZIELSKI, J.: How much to the ion-dipole capture rate constants obtained by transition state theory differ from those given by trajectory calculations?, **67**, 181
TUTCHER, B., *see* Ashfold, M.N.R.
TYUTEREV, V.G., CHAMPION, J.P., and PIERRE, G.: Reduced effective Hamiltonians for degenerate excited vibrational states of tetrahredral molecules: application to $2\upsilon_2$, $\upsilon_2 + \upsilon_4$ and $2\upsilon_4$ of CH_4, **71**, 995

UBACHS, W., *see* Aben, I.
UGOZZOLI, F., *see* Maniero, A.L.
ULSTRUP, J., *see* Hansen, W.N.
ULIVI, L., *see* Bafile, J.
ULIVI, L., *see* El-Sheikh, S.M.
UMANSKII, S., YA., *see* Nikitin, E.E.
UMANSKII, I.M., *see* Vetchinkin, S.I.
URBAN, W., *see* Bachem, E.
URBAN, W., *see* Havenith, M.
URBAN, W., *see* Huhn, B.
URBAN, W., *see* Lipus, K.
URBAN, W., *see* Nelis, Th.
URBAN, W., *see* Petri, M.
URBAN, W., *see* Seebas, W.
URBAN, W., *see* Simon, U.
URBAN, W., *see* Stackmann, V.
URBAN, W., *see* Towle, J.P.
URBAN, W., *see* Zimmermann, W.
URRECHA, , I., and ITURBE, J.: Quasiclassical trajectory study of the F + ICl system: effect of the triplet energy of IF, **75**, 763
URSU, I., BOGDAN, M., FITORI, P., BALIBANU, F., and DEMCO, D.E.: ^{19}F-^{235}U scalar interaction in liquid UF_6 by N.M.R. relaxation in the rotating frame, **62**, 793
USENKO, A.S.: Equilibrium distribution functions for plasma-molecular layers, **71**, 721
USENKO, A.S., and ZAGORODNY, A.G.: Brownian particle motion in a system with absorbing boundaries, **61**, 1213
UTRERA, L., *see* Böhm, M.C.

VALA, M., *see* Pellow, R.
VALENTIN, A., *see* Lattanzi, F.
VALENTIN, A., *see* Perrin, A.
VALLAURI, R., *See* Bertolini, D.
VALLAURI, R., *see* Steele, W.A.
VALYAEV, V.I., MOLIN, YU. N., SAGDEEV, R.Z., HORE, P.J., MCLAUCHLAN, K.A., and SIMPSON, N.J.K.: Cross relaxation in free radicals with chemically induced electron and nuclear polarization, **63**, 891
VAN AERT, A.H.J.M.; *see* Wang, D.M.
VAN BELL, D., FROEYEN, M., LIPPENS G., and WODAK, S.J.: Molecular dynamics simulation of polarizable water by an extended Lagrangian method, **77**, 239
VAN BELLE, D., *see* Lippens, G.
VAN BELLE, D., *see* Prevost, M.

VAN DAM, T., *see* McCourt, F.R.W.
VANDER AUWERA, J., *see* Herman, M.
VANDER AUWERA, J., *see* Abbouti Temsamani, M.
VAN DER EERDEN, J.P., *see* Groot, R.D.
VAN DER LUGT, W., *see* van der Marel, C.
VAN DER MAREL, C., BRAS, W., and VAN DER LUGT, W.: X-ray diffraction measurements on liquid iodine and some dilute mixtures of KI in I_2, **64**, 445
VAN DER MAREL, C., BRAS, W., and VAN DER LUGT, W.: X-ray diffraction measurements on liquid iodine and some dilute mixtures of KI in I_2 (erratum), **66**, 863
VAN DER MIJDEN, J.A.M., JANSSEN, R., and VEEMAN, W.S.: Analytical description of the $I^{-5}/_2$ quadropole nutation experiment, **69**, 53
VAN DER POL, A., REIJERSE, E.J., DE BOER, E., WASOWICZ, T., and MICHALIK, J.: The electron paramagnetic resonance spectrum of Ag_3^{2+}, **75**, 37
VAN DER WAALS, J.H., *see* Barendswaard, W.
VAN DER WAALS, J.H., *see* Van Tol, J.
VAN DER ZWAN, G., *see* Aben, I.
VAN DUIJNEN, P. TH., *see* Rullmann, J.A.C.
VAN DUIJNEVELDT, F.B., *see* Gutowski, M.
VAN DUIJNEVELDT, J.S., *see* Lynden-Bell, R.M.
VAN DUIJNEVELDT, F.B., *see* McCourt, F.R.W.
VAN DUIJNEVELDT, F.B., *see* Vos, R.J.
VAN EIJK, C.W.E., *see* Andriessen, J.
VAN HULST, J.A., *see* Van Tol, J.
VAN KOEVEN, D., *see* Brocks, G.
VAN LENTHE, J.H., VERBEEK, J., and PULAY, P.: Convergence and efficiency of the valence bond self-consistent field method, **73**, 1159
VAN LENGTHE, J.H., *see* Vos, R.J.
VAN LEEUWEN, J.M.J., *see* Nijmeijer, M.J.P.
VAN LEEUWEN, M.E., SMIT, B., and HENDRIKS, E.M.: Vapour-liquid equilibria of Stockmayer fluids. Computer simulations and perturbation theory, **78**, 271
VAN NHU, N., *see* Kohler, F.
VAN ORDEN, A., *see* Hwang, H.J.
VAN SWOL, F., *see* Courtemanche, D.J.
VAN SWOL, F., *see* de Miguel, E.
VAN SWOL, F., *see* Heffelfinger, G.S.
VAN SWOL, F., *see* Jackson, G.
VAN SWOL, F., *see* Marconi, U.M.B.
VAN SWOL, F., *see* Tan, Z.
VAN TASSEL, P.R., DAVIS, H.T., and MCCORMICK, A.V.: Monte Carlo calculations of adsorbate placement and thermodynamics in a micropore: Xe in NaA, **73**, 1107
VAN TASSEL, P.R., DAVIS, H.T., and MCCORMICK, A.V.: Monte Carlo calculations of Xe arrangement and energetics in the NaA alpha cage, **76**, 411
VAN TOL, J., *see* Barendswaard, W.
VAN TOL, J., VAN HULST, J.A., and VAN DER WAALS, J.H.: The luminescent triplet state of VO_4^{3-} in YPO_4. I. Polarization of the emission, **76**, 547
VAN TOL, J., and VAN DER WAALS, J.H.: The luminescent triplet state of VO_4^{3-} in YPO_4. II. Electron paramagnetic resonance and ^{51}V electron nuclear double resonance, **76**, 567
VANQUICKENBORNE, L.G., *see* Nguyen, M.T.
VARANDAS, A.J.C., *see* Matias, M.A.
VARANDAS, A.J.C., and PAIS, A.A.C.C.: A realistic double many-body expansion (DMBE) potential energy surface for ground-state O_3 from a multiproperty fit to *ab initio* calculations, and to experimental spectroscopic, inelastic scattering, and kinetic isotope thermal rate data, **65**, 843
VARDAG, T., *see* Speedy, R.J.
VAREA, C., *see* Romero-Rochin, V.
VARIYAR, J.E., and KIVELSON, D.: A molecular dynamics study of structure and dynamics in high-density liquids. II. Three dimensions, **79**, 235

VASI, C., *see* Magazú, S.
VASI, C., *see* Maisano, G.
VASI, C., *see* Majolino, D.
VASQUEZ, S.O., *see* Acevedo, R.
VASUDEVAN, V.J., *see* Elliott, J.R. Jr.
VASUDEVAN, V.J., and ELLIOTT, J.R., JR.: Structure and thermodynamics of chain molecular fluid mixtures, **75**, 443
VAQUEZ, L., and RIOS, M.A.: Geometrical distortion caused by substituents. II. A theoretical model for the analysis of its distribution, **65**, 129
VECCHIOCATTIVI, F., *see* Aguilar, A.
VEEMAN, W.S., *see* van der Mijden, J.A.M.
VEGA, C., *see* Boublik, T.
VEGA, C., *see* López Rodriguez, A.
VEGA, C., *see* Padilla, P.
VEGA, C., *see* Paras, E.P.A.
VEGA, C.: A perturbation theory of hard quadrupolar fluids, **75**, 427
VEGA, C., and FRENKEL, D.: Monte Carlo study of rod-like molecules. A test of perturbation theory for the Kihara model, **67**, 633
VEGA, C., and GUBBINS, K.E.: Monte Carlo study of quadrupolar Kihara fluids, **75**, 881
VEGA, C., and LAGO, S.: Structural study of the angle-averaged soft Kihara potential for linear molecular models. A test of perturbation theory, **72**, 215
VEGA, C., SAAGER, B., and FISCHER, J.: Molecular dynamics studies for the new refrigerant R152a with simple model potentials, **68**, 1079
VEGA, S., *see* Frydman, L.
VEGA, S., *see* Zaborowski, E.
VEGIRI, A., and FARANTOS, S.C.: A classical dynamical investigation of the mechanism of electronic quenching of OH($A\ ^2\Sigma^+$) in collisions with CO($X\ ^1\Sigma^+$), **69**, 129
VEGUILLAS, J., *see* Diaz, M.A.
VELARDE, J.M., PINERO, P., RULL, L.F., and MORALES, J.J.: Dependence of the critical thermodynamic variables on the shape of the potential, **65**, 287
VELASCO, S., *see* Hernández, A.C.
VELASCO, S., CALVO HERNANDEZ, A., GUEMEZ, J., PEREZ, J. and WHITE, J.A.: Numerical study of T_1 and T_2 rotational relaxation times of HCl in liquid Ar, **65**, 413
VELINO, B., *see* Caminati, W.
VENANZI, M., *see* Gianturco, F.A.
VENUTO, S., *see* Maisano, G.
VERBEEK, J., *see* Van Lenthe, J.H.
VERDASCO, E., SAEZ RABANOS, V., AOIZ, F.J., and GONZALEZ URENA, A.: Influence of the radical group upon total reaction cross section molecular beam study of the K + $RI \rightarrow$ KI + R (R = CH_3, C_2H_5, C_3H_7) reactions, **62**, 1207
VERGES, J., *see* Amiot, C.
VERGES, J., *see* Bernard, A.
VERGES, J., *see* Effantin, C.
VERGES, J., *see* Fellows, C.E.
VERGES, J., *see* Gustavsson, T.
VERMESSE, J., and LEVESQUE, D.: Simulations of adsorption on microporous interfaces, **77**, 837
VERMESSE, J., *see* Vidal, D.
VERSMOLD, H., *see* Härtl, W.
VERSMOLD, H. *see* Reh, M.
VERVLOET, M.: Study of the electronic ground state NH_2 by laser excited fluorescence Fourier transform spectroscopy, **63**, 433
VERVLOET, M., *see* Dabrowski, I.
VERVLOET, M., *see* Hemmerling, B.
VERVLOET, M., *see* Herman, M.
VERVLOET, M., *see* Huber, K.P.
VERLET, L., *see* Levesque, D.

VESELY, F.J., *see* Flener, P.
VESELY, F.J., and POSCH, H.A.: Correlated motion of 2 particles in a fluid. I. Stochastic equation of motion, **64**, 97
VESOVIC, V., *see* McCourt, F.R.W.
VESOVIC, V., and WAKEHAM, W.A.: An interpretation of intermolecular pair potentials obtained by inversion for non-spherical systems, **62**, 1239
VETCHINKIN, S.I., BAKHRAKH, V.L., and UMSANSKII, I.M.: Two-photon multiterm non-adiabatic transitions. I. WKB theory of resonance Raman scattering, **66**, 1139
VETCHINKIN, S.I., BAKHRAKH, V.L., IEVLEVA, L.D., and POPOV, A.F.: Two-photon multi-term nonadiabatic transitions. I. The resonance Raman scattering via the predissociation state, **66**, 1157
VIDAL, D., GUENGANT, L., MALBRUNOT, P., and VERMESSE, J.: Dielelectric constant of dense krypton at moderate densities and at three temperatures, **68**, 737
VIEHLAND, L.A., *see* Iinuma, K.
VIGUE, J., *see* Gouédard, G.
VIGUE, J., *see* Zalicki, P.
VIJ, J.K., *see* Corcoran, P.M.
VIJ, J.K., GROCHULSKI, T., KOCOT, A., and HUFNAGEL, F.: Complex permittivity measurements of acetone in the frequency region 50-310 GHz, **72**, 353
VIJAYARAGHAVAN, D., *see* McDonald, P.J.
VILLARRAL, P., *see* Gouédard, G.
VILLAVERDE, A., *see* Castillo, R.
VIOLA, L., *see* Iachello, F.
VIOT, P., *see* Tarjus, G.
VIQUE, J., *see* Billy, N.
VIQUE, J., *see* Gouédard, G.
VISCIDO, L., *see* Heras, J.M.
VISHWAMITTAR, *see* Srivastava, S.
VLADIMIROFF, T., CARIGNAN, Y.P., MACPHERSON, A.K., and MACPHERSON, P.A.: The dynamics of hard spheres in a collapsing spherical container, **71**, 441
VOGELSANG, R., HOHEISEL, G., and LUCKAS, M.: Shear viscosity and thermal conductivity of the Lennard-Jones liquid computed using molecular dynamics and predicted by a memory function model for a large number of states, **64**, 1203
VOGELSANG, R., *see* Schindler, H.
VOIGT, E.-M., *see* Chen, W.-H.
VOIT, B., *see* Franzke, D.
VOITLÄNDER, , J., *see* Trentini, F.V.
VOJTIK, J., *see* Polák, R.
VOLD, R.L., *see* Greenfield, M.S.
VOLOSHIN, V.P., *see* Naberukhin, Y.I.
VON BORCZYSKOWSKI, C.: Phosphorescence, ODMR and ODNQR investigation of the distorted lowest excited triplet state of symtetrachloropyrazine, **61**, 645
VON DREELE, R., *see* Torrie, B.H.
VON MALTZAN, B., *se* Jaegermann, P.
VON NAGY-FELSOBUKI, E.I., *see* Wang, F.
VON NIESSEN, W., *see* Tomasello, P.
VON PUTTKAMER, K., and QUACK, M.: High resolution interferometric FTIR spectroscopy of $(HF)_2$: analysis of a low frequency fundamental near 400 cm^{-1}, **62**, 1047
VON PUTTKAMER, K., QUACK, M., and SUHM, M.A.: Observation and assignment of tunnelling-rotational transitions in the far infrared spectrum of $(HF)_2$, **65**, 1025
VORONIN, A.I., *see* Osherov, V.I.
VORONKOVA, V.K., MOSINA, L.V., YABLOKOV, YU. V., KOVACIK, I., LANGFELDEROVA, H., and KOZISEK, J.: Effects of low symmetry and spin-spin interaction in the centrosymmetric dimer $[Cu(PU)_3(ClO_4)_2]_2$ with out-of-plane bond, **75**, 1275
VORTLER, H.L., KILAFA, J., and NEZBEDA, I.: Computer similation studies of hard body fluid mixtures, II, **68**, 547

VOS, I., *see* Ceulemans, R.
VOS, R.J., VAN DUIJNEVELDT, F.B., and VAN LENTHE, J.H.: Balance in interaction energy calculations. Counterpoise procedure in configuration space for the ICF method applied to the He-dimer, **67**, 1011
VOSTRIKOVA, N.G., *see* Brilliantov, N.V.
VRABEC, J., *see* Lotfi, A.

WAGNIÈRE, G., *see* Woźniak, S.
WAISMAN, E.M., *see* Pastore, G.
WAKEHAM, W.A., *see* Cole, W.A.
WAKEHAM, W.A., *see* Maitland, G.C.
WAKEHAM, W.A., *see* McCourt, F.R.W.
WAKEHAM, W.A., *see* Vesovic, V.
WAKITA, H., *see* Ichikawa, K.
WALDECK, J.R., *see* Black, J.F.
WALES, D.J., Hybridization schemes for clusters, **67**, 303
WALES, D.J.: Coexistence in small inert gas clusters, **78**, 151
WALES, D.J. Theoretical study of some small van der Waals complexes containing inert gas atoms, **74**, 1
WALES, D.J., *see* Stone, A.J.
WALKER, E.C., CHRISTIANSEN,P.A., and PACIOS, L.F.: Orbital partitioning errors in transition metal relativistic effective potentials, **63**, 139
WALKER, K.A., HEDDERICH, H.G., and BERNATH, P.F.: High resolution vibration-rotation emission spectroscopy of BaH, **78**, 577
WALLQVIST, A., *see* Ahlström, P.
WALLQVIST, A., and TELEMAN, O.: Properties of flexible water models, **74**, 515
WALRAND, J., *see* Dang-Nhu, M.
WALSH, J., *see* Tanaka, H.
WALSH, J.M., and GUBBINS, K.E.: The liquid structure and thermodynamic properties of Lennard-Jones spheres with association sites, **80**, 65
WALTERS, S.G., PENOTTI, F, GERRAT, J., and RAIMONDI, M.: Study of the mechanism of formation of $CH_2^+(^2A_1, {}^2B_1)$ from $C^+(^2P) + H_2$ using spin-coupled valence bond theory, **61**, 1341
WALTHER, K.L., WOKAUN, A., and BAIKER, A.: Characterization of porous silica gels prepared via the sol-gel process by ^{29}Si CP/MAS solid-state NMR spectroscopy, **71**, 769
WANG, B.Y., CUMMINGS, P.T., and EVANS, D.J.: Nonequilibrium molecular dynamics study of molecular contributions to the thermal conductivity of carbon dioxide, **75**, 1345
WANG, C.H., ZHU, X.R., and SHEN, J.C.: Angular and temperature dependence of depolarized and polarized Rayleigh-Brillouin spectra of a supercooled liquid: o-terphenyl, **62**, 749
WANG, D.-C., *see* Dabrowski, I.
WANG, D.M., MEIJERS, S.M., and DE BOER, E.: Magnetic behaviour of $Fe(CN)_6^{3-}$ in surrounding of low symmetry studied by EPR, **70**, 1135
WANG, D.M., VAN AERT, A.H.J.M., and DE BOER, E. An E.P.R. study of Cr^{3+} in C_6H_4. COOH.COOK, **67**, 799
WANG, F., and von NAGY-FELSOBUKI, E.I.: Variational calculation of the ro-vibrational states of Na_3^+, **77**, 1197
WANG, J., *see* Gianotti, R.D.
WANG, J.Z., DAS, K.K., and BALASUBRAMANIAN, K.: Potential energy surfaces for insertion of Zr into H_2, **69**, 147
WANG, S.P., CHEN, A.F.T., and SCHWARTZ, M.: Rotational diffusion of tribromobenzene in solutions, **65**, 689
WANG, S.P., HU, W.P., and SCHWARTZ, M.: Raman bandshape of the degenerate υ_4 vibration and parallel rotational diffusion in CD_3I, **68**, 1125
WANNOUS, G., *see* Effantin, C.
WARD, D., and LADO, F.: Structure, thermodynamics and orientational correlations of the nematogenic hard ellipse fluid from the Percus-Yevick equation, **63**, 623
WARD, D.A., and LADO, F.: Percus-Yevick solutions for the planar dumbbell fluid, **64**, 1185

WASOWICZ, T., *see* Van der Pol, A.
WASSER, R., *see* Lounila, J.
WATANABE, K., ALLNATT, A.R., and MEATH, W.J.: Perturbation theory for the thermodynamic properties of liquid nitrogen using model potentials, **61**, 325
WATANUKI, I., *see* Yamazaki, T.
WATKINSON, T.M., *see* Lindberg, P.
WATSON, J.K.G.: The asymptotic asymmetric-top rotational partition function, **65**, 1377
WATSON, J.K.G.: Vibration-rotation Hamiltonians of linear molecules, **79**, 943
WATTS, P., *see* Lee, E.P.F.
WATTS, R.O., *see* Suhm, M.A.
WAUGH, K.C., *see* Millar, G.J.
WAZYNSKA, B., *see* Imbardelli, D.
WEBER. J., and WOKAUN, A.: Two-dimensional NMR studies of the conformational B → Z transition in the oligodeoxynucleotides $d(CG)_8$ and $d(m^5CG)_8$, **74**, 293
WEBER, R.T., *see* Barendswaard, W.
WEDLER, G., *see* Ganzmann, I.
WEDLER, G., *see* Heras, J.M.
WEEKS, J.D., *see* Naidoo, K.J.
WEGDAM, G.H., and SCHAINK, H.M.: On the existence of sound propagation gaps in disparate mass gas mixtures, **65**, 531
WEIJNITZ, P., *see* Berg, L.-E.
WEIJNITZ, P., *see* Doverstål, M.
WEINER, J.H., *see* Gao, J.
WEIS, J.J., *see* Caillol, J.M.
WEIS, J.J., LEVESQUE, D., and ZARRAGOICOECHEA, G.J.: Singlet orientational distribution function and dielectric permittivity of dipolar sphereocylinders in the nematic phase, **80**, 1077
WEIS, J.J., *see* Zarragoicoechea, C.J.
WEISS, S.: Simulation of collision-induced absorption spectra rare-gas gaseous mixtures including ternary effects, **71**, 623
WEISS, S.: Simulation of gas phase collision-induced spectra and quadrupole-induced spectra including ternary effects, **72**, 987
WEISS, S.: Computer simulation of the vibrational spectrum of a simple system with ultrafast chemical reaction, **76**, 669
WELBERRY, T.R., *see* Baranyai, A.
WELKER, M., *see* Eggenberger, R.
WELLS, B.H.: van der Waals interaction potentials. Non-additivity in neon and argon lattices, **61**, 1283
WELLS, B.H., and WILSON, S.: van der Waals interaction potentials. Convergence of the many-body expansion, **65**, 1363
WELLS, B.H., and WILSON, S.: van der Waals interaction potentials. Many-body effects in Ne_4, **66**, 457
WELLS, G.B., YIM, M.G., and MAKINEN, M.W.: The influence of oxygen-17 enriched oxygen-donor ligands on the electronic spin relaxation behaviour of paramagnetic metal ions, **75**, 1285
WENDLAND, M., *see* Fischer, J.
WENDLAND, M., SALZMANN, S., HEINBUCH, U., and FISCHER, J.: Born-Green-Yvon results for adsorption of a simple fluid on plane walls. Structure, adsorption isotherms, and surface area determination, **67**, 161
WENG, S.-X., *see* Torrie, B.H.
WENG, S.-X., TORRIE, B.H., and POWELL, B.M.: The crystal structure of formaldehyde, **68**, 25
WENNERSTROM, H., *see* Granfeldt, M.
WENNERSTROM, H., *see* Westlund, P.-O.
WERNER, A., *see* Saricifi, N.S.
WERNER, J., *see* Havenith, M.
WERNER, J., *see* Seebass, W.
WESTERN, C.M., *see* Allen, J.M.
WESTERN, C.M., *see* Ashfold, M.N.R.

WESTLUND, P.-O., BENETIS, N., and WENNERSTROM, H.: Paramagnetic proton nuclear magnetic relaxation in the Ni^{2+} hexa-aquo complex. A theoretical study, **61**, 177
WESTLUND, P.-O., LARSSON, T.P., and TELEMAN, O.: Paramagnetic enhanced proton spin-lattice relaxation in the Ni^{2+} hexa-aquo complex. A theoretical and molecular dynamics simulation study of the Bloembergen-Morgan decomposition approach, **78**, 1365
WESTLUND, P.-O., *see* Halle, B.
WESTLUND, P.-O., *see* Laaksonen, A.
WESTLUND, P.-O., *see* Lynden-Bell, R.M.
WEYERICH, B., *see* Canessa, E.
WHALLEY, E., *see* Ikawa, S.
WHEATLEY, R.J.: Gaussian multipole functions for describing molecular charge distributions, **79**, 597
WHEATLEY, R.J., and MEATH, W.J.: On the relationship between first-order exchange and Coulomb interaction energies for closed shell atoms and molecules, **79**, 253
WHEATLEY, R.J., and MEATH, W.J.: Dispersion energy damping functions, and their scale with interatomic separation, for (H,He,Li)-(H,He,Li) interactions, **80**, 25
WHEATLEY, R.J., and PRICE, S.L.: An overlap model for estimating the anisotropy of repulsion, **69**, 507
WHEATLEY, R.J., and PRICE, S..: A systematic intermolecular potential method applied to chlorine, **71**, 1381
WHIFFEN, D.H.: Ensemble averages and molecular symmetry, **63**, 1053
WHITE, H.S., *see* Mier-y-Teran, L.
WHITE, H.S., *see* Zixiang Tang
WHITE, J.A., *see* Calvo Hernández, A.
WHITE, J.A., *see* Velasco, S.
WHITE, J.W., *see* Carlile, C.J.
WHITE, J.W., *see* Wielopolski, P.A.
WHITE, J.W., and WIELOPOLSKI, P.A.: Short wavelength collective excitations in graphite intercalate $C_{36}Cs$, **63**, 165
WHITE, J.W., and WIELOPOLSKI, P.A.: Effects of substrate potential on structure and dynamics of stage-3 graphite intercalated caesium, **63**, 669
WHITE, J.W., and WIELOPOLSKI, P.A.: Effects of substrate potential on structure and dynamics of stage-3 graphite intercalated caesium (erratum), **66**, 537
WHITE, R.W.P. *see* Jarvis, R.D.
WHITEHEAD, J.C., *see* Lindberg, P.
WHITHAM, C.J., *see* Sarre, P.J.
WHITLOCK, p., *see* Tawa, G.J.
WHITTLE, M., and MASTERS, A.J.: Liquid crystal formation in a system of fused hard spheres, **72**, 247
WHYMAN, G.E., *see* Mestechkin, M.M.
WIDOM, B., *see* Chatterjee, A.
WIDOM, B., *see* Perković, S.
WIDOM, B., *see* Szleifer, I.
WIELOPOLSKI, P.A., *see* Smith, E.R.
WIELOPOLSKI, P.A., and WHITE, J.W.: On the interaction potential of graphite intercalated alkali metals, **76**, 1281
WIELOPOLSKI, P.A., *see* White J.W.
WIELOPOLSKI, P.A., and WHITE, J.W.: Dynamics of the intercalated layer in $C_{36}Cs$: dependence on the temperature and substrate potential, **69**, 959
WIELOPOLSKI, P.A., WHITE, J.W., and HANLEY, H.J.M.: Structure of a stage-3 Cs-graphite intercalate, **69**, 947
WIESENFELD, L.: Effect of atomic number on parity-violating energy differences between enantiomers, **64**, 739
WIKLUND, S., *see* Magnusson, K.O.
WILDERS, A.E., *see* Lee, E.P.F.
WILKIE, J.M., *see* Randall, R.W.
WILLE, L.T.: Enumeration of normal hydrocarbon conformations, **61**, 409

WILLEMS, J.-P., CLEPHAS, M.P.J.W., and DE BOER, E.: EPR measurements on $K_3Co(CB)_6$ doped with $K_3Fe(CN)_6$: a determination of the polytype crystal structure of $K_3Co(CN)_6$, **80**, 607
WILLETTS, A., *see* Su, M-D.
WILLEY, D.R., BITTNER, D.N., and DE LUCIA, F.C.: Collisional cooling of the NO-He system. The pressure broadening cross sections between 4.3 and 1.8K, **67**, 455
WILLIAMS, C.P., *see* de Leeuw, S.W.
WILLIAMS, C.P., *see* Mooij, G.C.A.M.
WILLIAMS, C.P., *see* Smit, B.
WILLIAMS, G., *see* Jones P.
WILLIAMS, G., *see* Kozak, A.
WILLIAMS, I.H., *see* Francisco, J.S.
WILLIAMS, J.H.: An inelastic neutron scattering study of the dynamics of the van der Waals complex C_6H_6:C_6C_6, **73**, 99
WILLIAMS, J.H.: A quasielastic neutron scattering investigation of the van der Waals complex of benzene and hexafluorobenzene, **73**, 113
WILLIAMS, M.L., *see* Powles, J.G.
WILLIAMS, R.J.P.: Invited Article. Electron transfer in biology, **68**, 1
WILLIAMSON, J.M., *see* Liu, X.
WILSON, M.R., and ALLEN, M.P.: Computer simulation study of liquid crystal formation in a semi-flexible system of linked hard spheres, **80**, 277
WILSON, S.: The strong biorthogonality condition, **76**, 485
WILSON, S., and MONCRIEFF, D.: Can the ground state energy of H_2^+ be obtained to sub-microhartree accuracy with a basis set of s-type Gaussian functions?, **80**, 461
WILSON, S., *see* Wells, B.H.
WIMPERIS, S., and BODENHAUSEN, G.: Relaxation-allowed cross-peaks in two-dimensional N.M.R. correlation spectroscopy, **66**, 897
WIMPERIS, S., *see* Chung, Chun-Wa.
WIND, P., *see* March, N.H.
WINKEL, J.F., *see* Kenyon, A.J.
WINKELMANN, J., *see* Müller, A.
WINKLER, R.G., MORAWITZ, H., and YOON, D.Y.: Novel molecular dynamics simulations at constant pressure, **75**, 669
WINNEWISSR, G., *see* Saleck, A.H.
WINTER, H., *see* Lang, A.
WINTERTON, N., *see* Hall, C.D.
WINTHER, F., *see* Hegelung, F.
WLODARCZAK, G., DEMAISON, J., BURIE, J., and LASNE, M.C.: The rotational constants of acetylene-d, **66**, 669
WLODARCZAK, G., *see* Graner, G.
WODAK, S., *see* Prevost, M.
WODAK, S.J., *see* Lippens, G.
WODAK, S.J., *see* van Bell, D.
WOJCIECHOWSKI, K.W.: Constant thermodynamic tension Monte Carlo studies of elastic properties of a two-dimensional system of hard cyclic hexamers, **61**, 1247
WOJCIECHOWSKI, K.W.: Elastic constants of the hard disk system in the self-consistent free volume approximation, **72**, 955
WOJCIECHOWSKI, K.W., *see* Brańka, A.C.
WOKAUN, A., *see* Barnickel, P.
WOKAUN, A., *see* Franzke, D.
WOKAUN, A., *see* Kümmerlen, J.
WOKAUN, A., *see* Walther, K.L.
WOKAUN, A., *see* Weber, J.
WOKAUN, A., *see* Zimmermann, F.
WOLF,P., and MADER, H.: Pressure broadening of *Q*-branch rotational transition of germane by self-, H_2- and HCN collisions, **64**, 43

WOLIŃSKI, K., and SADLEJ, A.J.: Evaluation of the multipole-induced-multipole model: incremental dipole polarizabilities in the CH_4 ... He system, **75**, 221
WOLINSKI, K., SADLEJ, A.J., and KARLSTROM, G.: Molecular quadrupole moments, **72**, 425
WOLNIEWICZ, L., and ORLIKOWSKI, T.: The $1s\sigma_g$ and $2p\sigma_u$ states of the H_2^+, D_2^+ and HD^+ ions, **74**, 103
WOLNIEWICZ, L., and POLL, J.D.: On the higher vibration-rotational levels of HD^+ and H_2^+ (erratum), **66**, 701
WONG, A.T., BACKSAY, G.B., and HUSH, N.S.: *Ab initio* polarizability derivatives for methane: an application to Raman intensities of overtone and combination bands, **74**, 1037
WONG, A.T., and BACKSAY, G.B.: *Ab initio* potential energy surface and vibrational frequencies of HCN, **79**, 819
WONG, C.C.K., *see* Aziz, R.A.
WONG, C.C.K., *see* Hanson, E.E.
WONG, C.C.K., HANSON, E.E., and MCCOURT, F.R.W.: Classical trajectory calculation of transport and relaxation properties for CO_2-He mixtures, **74**, 497
WONG, C.C.K., MCCOURT, F.R.W., and DICKINSON, A.S.: A comparison between classical trajectory and infinite-order sudden calculations of transport and relaxation cross sections for N_2-Ne mixtures, **66**, 1235
WONG, C.C.K., MCCOURT, F.R.W., and COREY, G.C.: Classical trajectory calculation of transport and relaxation properties of O_2-He, Ne mixtures, **78**, 499
WOODS, G.B., PANAGIOTOPOULOS, A.Z., and ROWLINSON, J.S.: Adsorption of fluids in model zeolite cavities, **63**, 49
WOODWARD, C.E., *see* Svensson, Bo R.
WOODWARD, D.R., FLETCHER, D.A., and BROWN, J.M.: Dispersed fluorescence studies of the NCO radical. Fermi resonance between the (100) and (200) levels of the $X^2\Pi$ state, **62**, 517
WOODWARD, D.R., FLETCHER, D.A., and BROWN, J.M.: Dispersed fluorescence studies of the NCO radical. Fermi resonance between the (100) and (020) levels of the $X^2\Pi$ state (erratum), **68**, 261
WOOLF, L.A., *see* Harris, K.R.
WORNALD, C.J., *see* Adya, A.K.
WORMALD, C.J., *see* Howe, M.A.
WORMER, P.E.S., *see* Hettema, H.
WORMER, P.E.S., *see* Rijks, W.
WOŹNIAK, S.: Optically induced circular and axial birefringence and dichroism in molecular systems. I. Electric dipole and magnetic dipole transitions, **80**, 313
WOŹNIAK, S., EVANS, M.W., and WAGNIÈRE, G.: Optically induced static magnetization near optical resonance in molecular systems. 1. Inverse Faraday effect, **75**, 81
WOŹNIAK, S., EVANS, M.W., and WAGNIÈRE, G.: Optically induced static magnetization near optical resonances in molecular systems. 2. Inverse magnetochiral birefringence, **75**, 99
WRIGHT, J.S., *see* Baoqi Meng
WRIGHT, K.M., *see* Hills, B.P.
WRIGHT, P.E., *see* Palmer, A.G. III
WRIGHT, T.G., LEE, E.P.F., and DYKE, J.M.: Effects of BSSE and d-orbital space in the calculation of the equilibrium geometry of CaF_2, **73**, 941
WRIGHT, T.G., and LEE, E.P.F.: *Ab intio* studies of X_3 and X_3(X = F,Cl), **79**, 995
WRIGHT, T.G., *see* Lee, E.P.F.
WRZALIK, R., *see* Bródka, A.
WRZALIK, R., *see* Nikiel, L.
WU, X.-G., and BAUS, M.: Density functional theory for the freezing of charged hard spheres embedded in a uniform neutralizing background, **62**, 375
WULF, M., *see* Morgner, H.
WYATT, R.E., *see* Mohan, M.
WYTTENBACH, T., *see* Hanratty, M.A.

XIAO, C., and ROWLINDON, J.S.: The solvation pressure in a system of fixed density, **73**, 937

XIAO, W.Z., *see* Alden, R.G.
XIE, Y., *see* Quelch, G.E.
XIE, YAOMING, SCHAEFER, H.F., III, JANG, JEE HWAN, MHIN, BYUNG JIN, KIM, HO SOON, YOON, CHANG WOO and KIM, KWANG, S.: Sulfur clusters: structure, infrared, and Raman spectra of cyclo-S_6 and comparison with the hypothetical cyclo-O_6 molecule, **76**, 537
XU, H., and LYNDEN-BELL, R.M.: The onset of disorder on a surface with a step, **73**, 1401
XU, H.: A density functional study of nematic-smectic A-solid transitions of parallel hard sphereocylinders, **77**, 311

YABLOKOV, YU, V., *see* Voronkova, V.K.
YAKUB, E.S.: Integral equations for conventional functions of simple dimerizing fluids, **77**, 845
YAMADA, K.M.T., *see* Saleck, A.H.
YAMADA, T., CHUANG, T.J, SEKI, H., and MITSUDA, Y.: Chemisorption of fluorine, hydrogen and hydrocarbon species on the diamond C(111) surface, **76**, 887
YAMAGUCHI, T., *see* Ichikawa, K.
YAMAGUCHI, Y., *see* Quelch, G.E.
YAMANAKA, T., *see* Ichikawa, K.
YAMANOUCHI, K., *see* Brown, R.D.
YAMASHITA, A.B., *see* Sachiko Nakai
YAMAZAKI, T., OZAWA, S., and OGINO, Y.: Potential energies for methane adsorption in ion-exchanged ZSM-5 zeolite pore, **69**, 369
YAMAZAKI, T., WATANUKI, I., OZAWA, S., and OGINO, Y.: Potential energies and IR spectra for homopolar diatomic adsorbates over ion-exchanged ZSM-5 zeolites, **73**, 649
YAMAZAKI, T., KATOH, M., OZAWA, S., and OGINO, Y.: Absorption of CO_2 over univalent cation-exchanged ZSM-5 zeolites, **80**, 313
YANG, B., SULLIVAN, D.E., TJIPTO-MARGO, B., and GRAY, C.G.: Density-functional theory of the water liquid-vapour interface, **76**, 709
YAOMING XIE, *see* Tozer, DJ.
YARWOOD, G., *see* Chewter, L.A.
YARWOOD, G., *see* Smith, I.W.M.
YARWOOD, J., *see* Buchner, R.
YARWOOD, J., *see* Cabaço, M.I.
YARWOOD, J., *see* Guillaume, F.
YARWOOD, J., *see* Shelley, V.
YASHONATH, S., PRICE, S.L., and MCDONALD, I.R.: A six-site anisotropic atom-atom potential model for the condensed phases of benzene, **64**, 361
YASHONATH, S., and SANTIKARY, P.: Influence of non-geometrical factors on intracrystalline diffusion. Role of sorbate-zeolite interactions, **78**, 1
YATES, B.F., *see* Quelch, G.E.
YENCHA, A.J., *see* Kvaran, A.
YENICE, K.M., LEE, S.A., and DOWNS, D.W.: Optical properties of methanol at high pressures, **69**, 973
YEOMANS, J.M., *see* Dobbs, H.T.
YERSIN, H., *see* Braun, D.
YETHIRAJ, A., and HALL, C.K.: Square well diatomics: bulk equation of state, density profiles near walls, virial coefficients and coexistence properties, **72**, 619
YETHIRAJ, A., and HALL, C.K.: Monte Carlo simulation of the equilibrium partitioning of chain fluids between a bulk and a pore, **73**, 503
YETHIRAJ, A., and HALL, C.K.: On equations of state for hard chain fluids, **80**, 469
YETHIRAJ, A.: Local structure of tangent-hard-sphere diatomic fluids, **80**, 695
YIM, M.B., *see* Wells, G.B.
YONGFANG ZHAO, *see* Pyykkö, P.
YOON, B.J., *see* Hong, S.D.
YOON, CHANG WOO, *see* Xie, Yaoming.
YOON, D.Y., *see* Winkler, R.G.

YOSHIMINE, M., *see* Minh Tho Nguyen
YOSHIMURA, Y., *see* Kimura, Y.
YOUNG, N.A., *see* Beattie, I.R.
YOUNG, P., GREEN, D.V.S., HILLIER, I.H., and BURTON, N.A.: Assessment of quantum mechanical continuum models of solvation: the prediction of tautomer equilibria, partition coefficients and amine basicity, **80**, 503
YOUNG, S.H., and KUKOLICH, S.G.: Molecular hyperfine-structure calculations using an uncoupled representation, **71**, 181
YOUNG, W.H., *see* Hoshino, K.
YU, J.-T., and CHOU, S.Y.: E.S.R. of gamma-irradiated $LiCsSO_4$ crystals doped with NH_4^+, **62**, 971
YU, J., *see* Liu, X.

ZABOROWSKI, E., and VEGA, S.: A study of Dianin's inclusion compound. NMR and energy calculations, **78**, 703
ZACHILAS, L., *see* Farantos, S.C.
ZACKRISSON, M., *see* Launila, O.
ZAGORODNY, A.G., *see* Usenko, A.S.
ZAHAB, A., *see* André, D.
ZALICKI, P., BILLY, N., GOUÉDARD, G., and VIGUE, J.: Coherent saturation effects in a Na_2 laser-induced fluorescence experiment: theory and experiment, **79**, 899
ZANASI, R., *see* Fowler, P.W.
ZANASI, R., *see* Lazzeretti, P.
ZANASI, R., *see* Raynes, W.T.
ZANNONI, C., *see* Arcioni, A.
ZANNONI, C., *see* Biscarini, F.
ZANNONI, C., *see* Chiccoli, C.
ZARE, R.N., *see* Black, J.F.
ZARE, R.N., *see* Nagata, T.
ZARE, R.N., *see* Zhao, D.
ZARRAGOICOECHEA, G.J., LEVESQUE, D., and WEIS, J.J.: Monte Carlo study of dipolar ellipsoids. I. The isotropic phase, **74**, 629
ZARRAGOICOECHEA, G.J., LEVESQUE, D., and WEIS, J.J.: Monte Carlo study of dipolar ellipsoids. II. Search for an isotropic-nematic phase transition, **75**, 989
ZARRAGOICOECHEA, G.J., LEVESQUE, D., and WEIS, J.J.: Monte Carlo simulations of polar discotic molecules, **78**, 1475
ZARRAGOICOECHEA, G.J., *see* Weis, J.J.
ZEIDLER., M.D., *see* Gordalla, B.C.
ZEIDLER, M.D., *see* Jung, W.G.
ZEIDLER, M.D., *see* Meckl, S.
ZEIDLER, M.D., *see* Mittag, U.
ZEIDLER, M.D., *see* Neuefeind, J.
ZEMKE, K., SCHMIDT-ROHR, K., MAGIL, J.H., SILLESCU, H., and SPIESS, H.W.: Molecular dynamics near the glass transition. A two-dimensional ^{13}C NMR study of 1,3,5-tri-α-naphthylbenzene, **80**, 1317
ZERBETTO, F., *see* Caminati, W.
ZERDA, T.W., *see* Brodka, A.
ZHANG, M.Q., *see* Percus, J.K.
ZHANG, Q., and BADIALI, J.P.: Optical birefringence in inhomogeneous polar liquids. Existence of a natural Kerr effect, **75**, 325
ZHANG, X., *see* Li, Q.
ZHANG, Z.C., and PYPER, N.C.: Exact relativistic analogues of the non-relativistic hyperfine structure operators. II. A numerical study, **64**, 963
ZHANG, Z., ZUCKERMANN, M.J., and MOURITSEN, O.G.: Phase transition and director fluctuations in the three-dimensional Lehwohl-Lasher model of liquid crystals, **80**, 1195
ZHAO, D., and ZARE, R.N.: Numerical computation of 9-*j* symbols, **65**, 1263

ZHAO, Y., *see* Francisco, J.S.
ZHAO, Y., and FRANCISCO, J.S.: The vibrational spectrum of FBrCO. An experimental and theoretical study, **77**, 1187
ZHAO, Y., and FRANCISCO, J.S.: Infrared photochemistry of FBrCo. An experimental and theoretical study, **79**, 1
ZHELYASKOV, V., GEORGIEV, G., NICKOLOV, ZH., and MITEVA, M.: Concentration Raman study of intramolecular, intermolecular and Fermi resonance interactions in the OH stretching spectra of dilute solutions of HDO and D_2O using Fourier deconvolution technique, **64**, 1133
ZHEN, J., *see* Larsen, S.Y.
ZHILINSKII, B.I., *see* Sadovskii, D.A.
ZHOU, Y., and STELL, G.: Fluids inside a pore - an integral-equation approach. I. General formalism and hard spheres inside spherical and slit pores, **66**, 767
ZHOU, Y., and STELL, G.: Fluids inside a pore - an integral-equation approach. II. Cylindrical pores, **66**, 791
ZHOU, Y., and STELL, G.: Fluids inside a pore - An integral equation approach, III. Water-in-oil microemulsions, **68**, 1265
ZHU, J.-B., *see* Zhu, S.-B.
ZHU, S.-B., LEE, J., and ROBINSON, G.W.: Molecular dynamics simulation of liquid carbon disulphide with a harmonic intramolecular potential, **65**, 65
ZHU, S.-B., LEE, J., and ROBINSON, G.W.: Structure and properties of liquid carbon disulphide near extended surfaces, **67**, 321
ZHU, S.-B., ZHU, J.-B., and ROBINSON, G.W.: Structure and properties of liquid carbon disulphide between charged plates, **68**, 1321
ZHU, X.R., *see* Wang, C.H.
ZHU. Z.Z., *see* Jarvis, R.D.
ZIMMERMAN, D.S., and BURNELL, E.E.: Size and shape effects on the orientation of solutes in nematic liquid crystals, **69**, 1059
ZIMMERMAN, D.S., and BURNELL, E.E.: Anisotropic short range potentials for solutes in nematic liquid crystals, **78**, 687
ZIMMERMAN, D.S., *see* Li, K.Y.
ZIMMERMAN, D.S., *see* Ter Beek, L.C.
ZIMMERMANN, F., and WOKAUN, A.: Giant gold clusters stabilized by triphenylphospine ligands. Characterization by surface enhanced Raman and reflectance spectroscopy, **73**, 949
ZIMMERMANN, H., *see* Bernhard, T.
ZIMMERMANN, H., *see* Filsinger, B.
ZIMMERMANN, H., *see* Idziak, S.
ZIMMERMANN, W., *see* Huhn, B.
ZIMMERMANN, W., *see* Petri, M.
ZIMMERMANN, W., *see* Simon, U.
ZIMMERMANN, W., NELIS, TH., BACHEM, E., PAHNKE, R., and URBAN, W.: The infrared L.M.R. spectrum of SnH, **68**, 199
ZIMMERMANN, W., SIMON, U., PETRI, M., and URBAN, W.: The observation of fine-structure transitions in the SnH radical by diode laser spectroscopy, **74**, 1287
ZIMMERMANN, W., SMOLKA, K.-P., and URBAN, W.: Detection of the GeD($S^2\Pi$) vibration-rotation spectrum by laser magnetic resonance, **70**, 167
ZINK, L.R., *see* Burghardt, I.
ZIXIANG TANG, MIER-Y-TERAN, L., DAVIS, H.T., SCRIVEN, L.E., and WHITE, H.S.: Non-local free-energy density-functional theory applied to the electrical double layer. Part I: Symmetrical electrolytes, **71**, 369
ZOLLWEG, J.A., *see* Holcomb, C.D.
ZOLLWEG, J.A., *see* Johnson, J.K.
ZOLLWEG, J.A., *see* Shaoyi, Jiang
ZOPPI, M., *see* Bafile, U.
ZUCKERMANN, M.J., *see* Zhang, Z.
ZULICKE, L., *see* Schneider, F.
ZUNIGA, J., *see* Requena, A.

ZWOLINSKI, B.J., *see* Pas, M.F.

Issued free of charge to subscribers to *Molecular Physics*, with Volumes 84, 85 and 86 (1995)